Supporting Information

Phosphoramidite Gold(I)-Catalyzed Diastereo- and Enantioselective Synthesis of 3,4-Substituted Pyrrolidines

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1. General Information

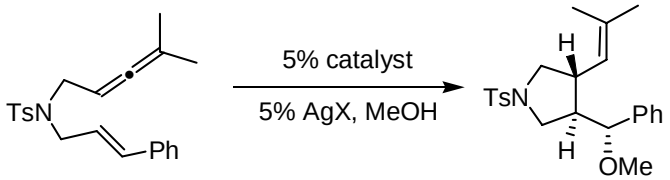
Unless otherwise noted, all reagents were obtained commercially and used without further purification. All reaction mixtures excluding the gold(I)-catalyzed reaction mixtures were stirred with a magnetic stir bar in flame-dried glassware under a nitrogen atmosphere. Tetrahydrofuran (THF), diethyl ether (Et_2O) and dichloromethane (CH_2Cl_2) were dried by passing commercially available pre-dried, oxygen-free formulations through activated alumina columns. Triethylamine (Et_3N) was distilled from CaH_2.[1] Dry DMSO and DMF were obtained from Acros. Extracts were dried over $MgSO_4$ and solvents were removed in a rotary evaporator. TLC analysis of reaction mixtures was performed on Merck silica gel 60 F254 TLC plates. Unless otherwise indicated, chromatography was carried out on ICN SiliTech 32-63 D 60Å silica gel. ^1H, ^{13}C, and ^{31}P NMR spectra were recorded with Bruker AMX-300, AVQ-400, AVB-400, DRX-500 and AV-500 spectrometers and referenced to $CDCl_3$, CD_2Cl_2 or C_6D_6. Structures were confirmed using NOESY, COSY and HSQC experiments. Mass spectra data were obtained at the Micro-Mass/Analytical Facility in the College of Chemistry, University of California, Berkeley.

[1] Alaimo, P.J.; Peters, D.W.; Arnold, J.; Bergman, R.G. *J. Chem. Ed.* **2001**, *78*, 64.

2. Selected Analytical Data and Representative Experimental Procedures.

2.1 Additional Results

Table 1. Additional Catalysts Screened on the alkoxycyclization of 1b.

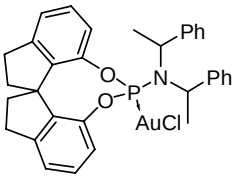


1b **3a**

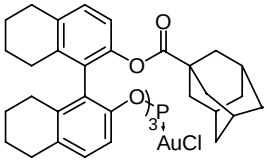
Entry	Catalyst	Solvent	Counterion (X)	% ee
1	*R*-**A**	DCM	BF_4	20
2	*S*-**B**	DCM	BF_4	14
3	(*S*,*S*,*S*)-**C**	DCM	BF_4	47
4	(*S*,*S*,*S*)-**D**	DCM	BF_4	14
5	(*S*,*S*,*S*)-**E**	DCM	BF_4	4
6	(*R*,*R*,*R*)-**F**	Nitromethane	BF_4	49
7	(*R*,*R*,*R*)-**G**	Nitromethane	BF_4	66
8	(*R*,*R*,*R*)-**H**	Nitromethane	BF_4	54
9	(*S*,*R*,*R*)-**I**	Nitromethane	BF_4	30
10	(*R*,*R*,*R*)-**I**	Nitromethane	BF_4	62
11	(*R*,*R*,*R*)-**J**	Nitromethane	BF_4	58
12[a]	(*R*,*R*,*R*)-**J**	Nitromethane	BF_4	72
13	(*R*,*S*,*S*)-**J**	Nitromethane	BF_4	28
14	(*R*,*R*,*R*)-**K**	Nitromethane	BF_4	32
15	(*S*,*S*,*S*)-**L**	Nitromethane	BF_4	30
16	(*R*,*R*,*R*)-**M**	Nitromethane	BF_4	58
17	[(*R*)-DTBM-SEGPHOS-Au_2][Cl]$_2$	DCM	BF_4	58

[a] Reaction run at 0°C.

Catalyst Leyend for Table 1:



A



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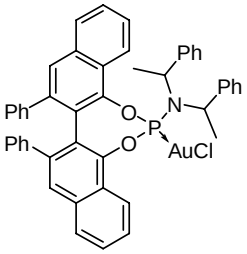

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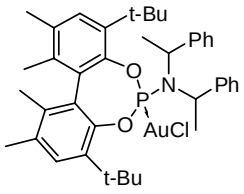

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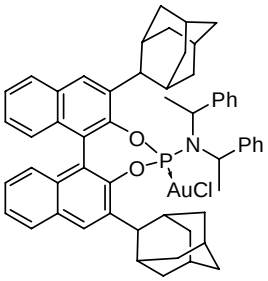

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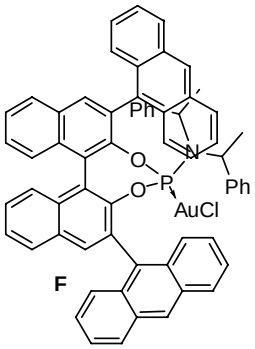

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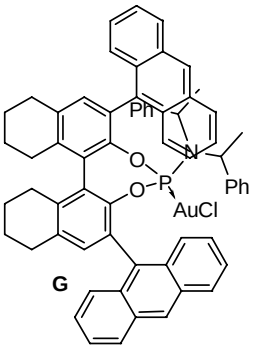

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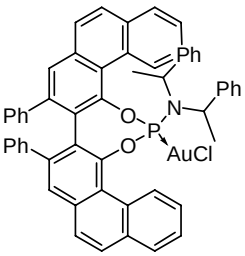

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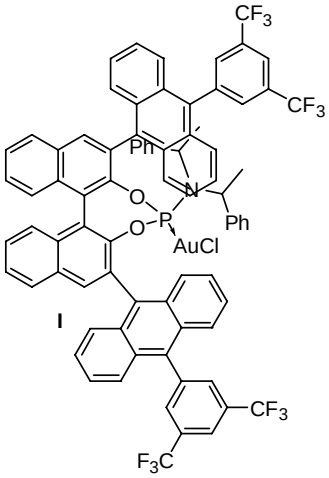

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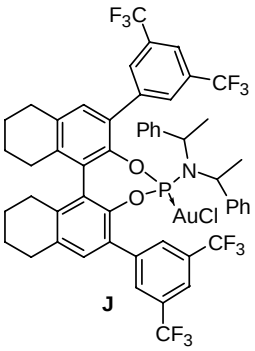

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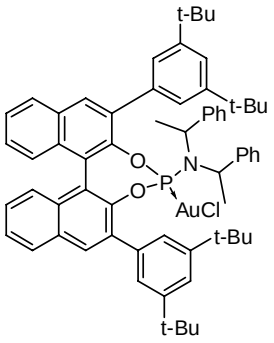

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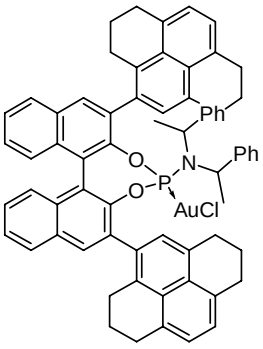
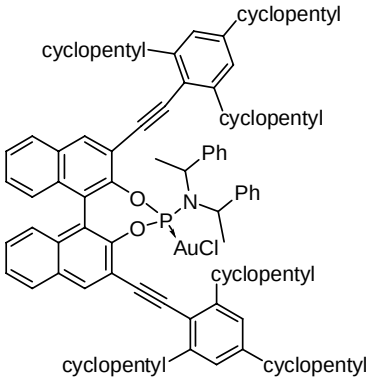
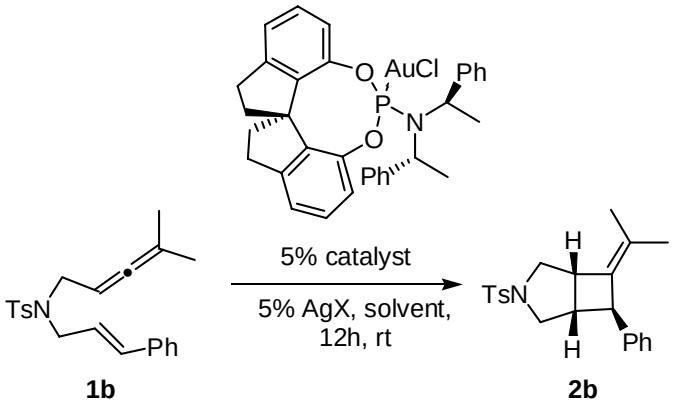


L



M

Table 2. Additional Conditions Screened for the [2+2]-cycloadditions of **1b** with (*R*,*R*,*R*)-**9a**.

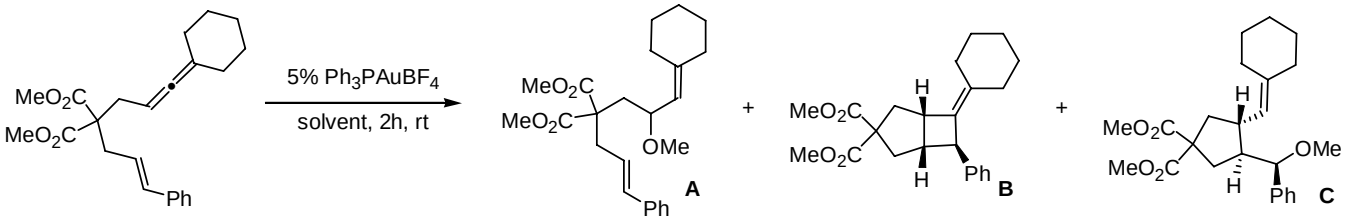


1b **2b**

Entry	Solvent	Counterion (X)	% yield	% ee
1	DCM	SbF_6	67	72
2	DCM	OTf	77	84
3	DCM	NTf_2	57	84
4	DCM	PF_6	64	52
5	DCM	NaBARF	31	90
6	DCM	BF_4	86	94
7	nitromethane	BF_4	34	66
8	dichloroethane	BF_4	57	66
9[a]	THF	BF_4	---	---
10	chloroform	BF_4	61	94
11[a]	chloroform	NaBARF	---	---

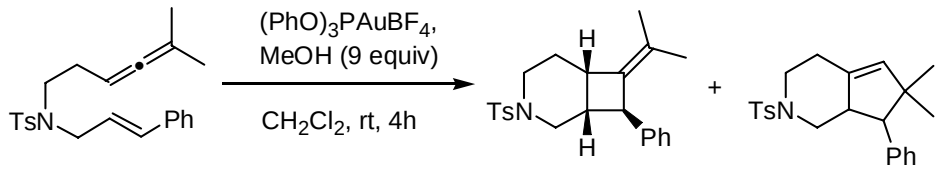
[a] No reaction at 35°C.

Table 3. MeOH trapping experiments.[b]



Entry	Solvent	A	B	C
1	MeOH	84[c]	---	---
2[a]	DCM	10	54	36 (32)[c]
3[a]	nitromethane	10	12	78 (70)[c]

[a] With 5 equiv. of MeOH. [b] Product distribution determined by ^{1}H NMR. [c] Isolated yield after silica gel column chromatography.

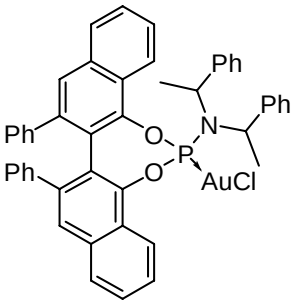


*For all phosphite and phosphoramidite tested this class of substrate gave us a mixture of the [2+2]- and [3+2]-cycloadducts.

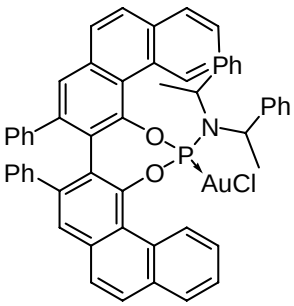
2.2 Preparation of Gold(I) Catalysts

Catalysts **5** and **6** were synthesized following previously reported literature procedures. All characterization data was in complete agreement with the reported values.[2]

Catalysts **7** and **8** were synthesized following previously reported literature procedures (see Footnote 2) from commercially available VANOL and VAPOL, respectively:

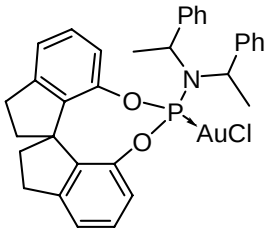


(*S*,*S*,*S*)-**7**. ^{1}H NMR (400MHz, $CDCl_3$): δ 8.13 (d, *J* = 8.6Hz, 1H), 7.91 (d, *J* = 7.5Hz, 1H), 7.59-7.47 (m, 8H), 7.25-6.88 (m, 16H), 6.51 (d, *J* = 7.2Hz, 2H), 6.35 (d, *J* = 7.2Hz, 2H), 5.08 (bs, 2H), 1.65 (s, 3H), 1.63 (s, 3H). ^{31}P NMR (162MHz, $CDCl_3$): δ 133.7.

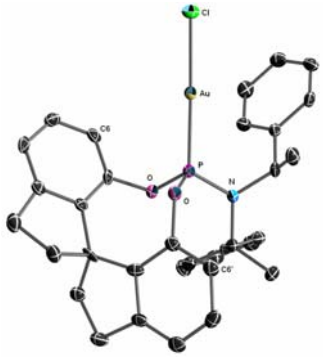


(*R*,*R*,*R*)-**8**. ^{1}H NMR (400MHz, $CDCl_3$): δ 9.62 (d, *J* = 8.0Hz, 1H), 8.07-8.05 (m, 2H), 7.95-7.89 (m, 2H), 7.82-7.75 (m, 4H), 7.68-7.64 (m, 3H), 7.56 (d, *J* = 1.2Hz, 1H), 7.33 (t, *J* = 8.0Hz, 1H), 7.20-6.87 (m, 16H), 6.71 (d, *J* = 7.2Hz, 2H), 6.41 (dd, *J* = 7.2, 1.2Hz), 5.04 (bs, 2H), 0.93 (s, 3H), 0.91 (s, 3H). ^{31}P NMR (162MHz, $CDCl_3$): δ 127.6.

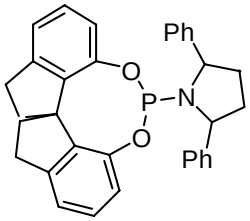
[2] (a) González, A. Z.; Toste, F. D. *Org. Lett.* **2010**, *12*, 200. (b) Alonso, I.; Trillo, B.; López, F.; Montserrat, S.; Ujaque, G.; Castedo, L.; Lledós, A.; Mascareñas, J. L. *J. Am. Chem. Soc.* **2009**, *131*, 13020.



Catalyst (*R*,*R*,*R*)-**9a** was synthesized from commercially available (*R*)-SIPHOS-PE (Sigma-Aldrich, 97% HPLC purity) via a modification of Puddephat pocedure (see bellow on the synthesis of **11c** for more details).[3] ^{1}H NMR (400MHz, $CDCl_3$): δ 7.24-6.99 (m, 16H), 4.60-4.53 (m, 2H), 3.18-3.06 (m, 2H), 2.93-2.82 (m, 2H), 2.38-2.33 (m, 1H), 2.23-2.19 (m, 1H), 2.13 (q, *J* = 10.8Hz, 1H), 2.07 (q, *J* = 10.8Hz, 1H). ^{31}P NMR (162MHz, $CDCl_3$): δ 116.2. See bellow structure of complex (*R*,*R*,R)-**9a**·AuCl in the solid state. Anisotropic displacement parameters are drawn at the 50% probability level and hydrogen atoms are omitted for clarity.

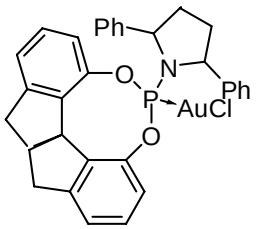


(*S*,*R*,*R*)-**9a** ^{1}H NMR (400MHz, $CDCl_3$): δ 7.20-7.09 (m, 14H), 6.64 (d, *J* = 8.0Hz, 1H), 6.58 (d, *J* = 8.0Hz, 1H), 4.98 (dq, *J* = 17.2, 6.8Hz, 2H), 3.14-3.01 (m, 2H), 2.90-2.81 (m, 2H), 2.27-2.16 (m, 2H), 1.96 (q, *J* = 11.6Hz, 2H), 1.51 (s, 3H), 1.49 (s, 3H). ^{31}P NMR (162MHz, $CDCl_3$): δ 118.3.

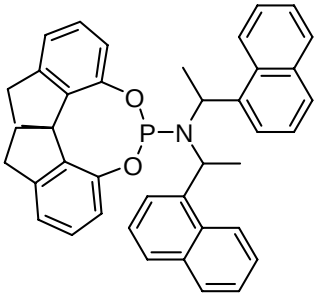


Synthezised from (*R*)-SPINOL[4] and commercially available (2*R*,5*R*)-diphenylpyrrolidine (Sigma-Aldrich) following the above-mentioned procedure.[2] ^{1}H NMR (400MHz, $CDCl_3$): δ 7.34-7.27 (m, 8H), 7.25-7.19 (m, 3H), 7.13 (d, *J* = 7.3Hz, 1H), 7.04 (t, *J* = 7.6Hz, 1H), 6.89 (d, *J* = 7.3Hz, 1H), 6.75 (d, *J* = 7.8Hz, 1H), 6.69 (d, *J* = 7.9Hz, 1H), 4.25 (bs, 2H), 3.08-2.91 (m, 2H), 2.84 (add, *J* = 15.8, 7.8Hz, 1H), 2.70 (add, *J* = 15.9, 8.0Hz, 1H), 2.31-2.28 (m, 2H), 2.15-2.08 (m, 2H), 1.88-1.72 (m, 4H). ^{31}P NMR (162MHz, $CDCl_3$): δ 129.1.

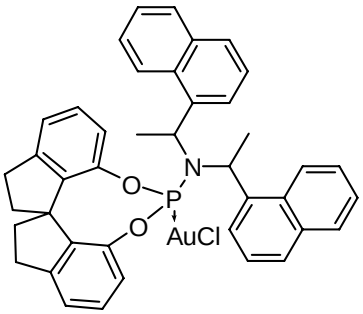
[3] Brandys, M.-C.; Jennings, M. C.; Puddephat, R. J. *Dalton* **2000**, 4601.
[4] Birman, V. B.; Rheingold, A. L.; Lam, K.-C. *Tetrahedron: Asymmetry*, **1999**, *10*, 125.



(*R*,*R*,*R*)-**9b**. Synthesized via a modification of Puddephat's pocedure.[3] ^{1}H NMR (400MHz, $CDCl_3$): δ 7.40-7.23 (m, 12H), 7.14 (t, *J* = 7.8Hz, 1H), 7.02 (d, *J* = 7.02Hz, 1H), 6.89 (d, *J* = 8.1Hz, 1H), 6.61 (d, *J* = 7.5Hz, 1H), 4.56 (bs, 2H), 3.12-2.93 (m, 2H), 2.87 (add, *J* = 16.1, 7.9Hz, 1H), 2.82 (add, *J* = 16.1, 7.9Hz, 1H), 2.48-2.44 (m, 2H), 2.28-2.10 (m, 2H), 1.97-1.92 (m, 2H), 1.89-1.81 (m, 1H), 1.78-1.66 (m, 1H). ^{31}P NMR (162MHz, $CDCl_3$): δ 112.7.

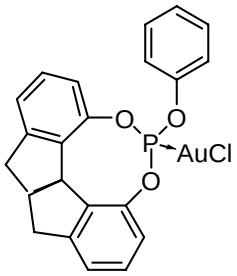


Synthezised from (*R*)-SPINOL[5] and the free-base of commercially available bis[(*R*)-(−)-(1-naphtyl)ethyl]amine hydrochloride (Sigma-Aldrich) following the above-mentioned procedure.[2] ^{1}H NMR (400MHz, $CDCl_3$): δ 7.95 (bs, 2H), 7.59 (d, *J* = 7.6Hz, 2H), 7.42-7.32 (m, 6H), 7.19 (t, *J* = 8.4Hz, 4H), 7.08 (d, *J* = 8.0Hz, 2H), 6.68 (bs, 2H), 5.46-5.41 (m, 2H), 3.26-3.05 (m, 2H), 3.98 (add, *J* = 16.0, 7.6Hz, 1H), 2.85 (add, *J* = 16.0, 7.5Hz, 1H), 2.33-2.23 (m, 2H), 2.18-2.13 (m, 1H), 2.04-1.99 (m, 1H), 1.26 bs, 6H). ^{31}P NMR (162MHz, $CDCl_3$): δ 132.7.



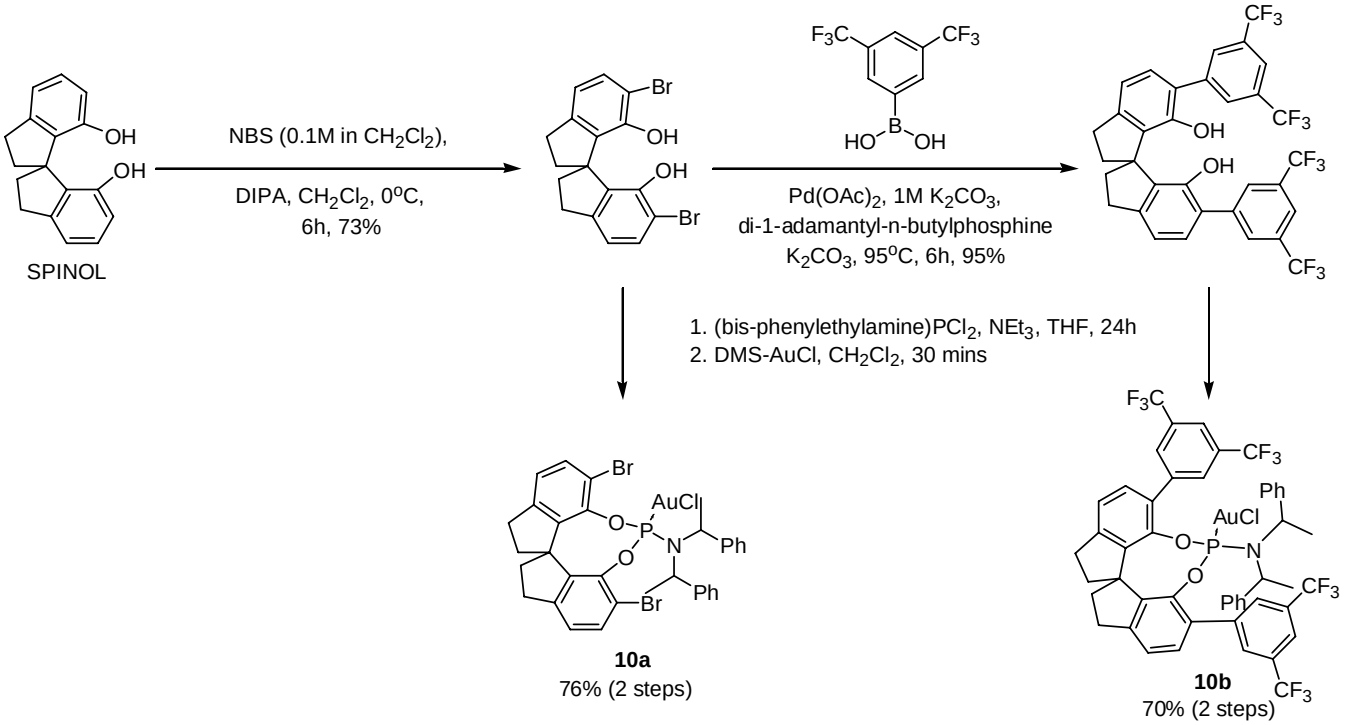
(*R*,*R*,*R*)-**9c**. Synthesized via a modification of Puddephat's pocedure.[3] ^{1}H NMR (400MHz, $CDCl_3$): δ 7.95 (d, *J* = 8.0Hz, 2H), 7.52-7.30 (m, 9H), 7.29-7.22 (m, 4H), 7.18 (d, *J* = 8.4Hz, 1H), 7.08 (d, *J* = 8.0Hz, 2H), 6.46 (t, *J* = 7.6Hz, 2H), 5.65-5.59 (m, 2H), 3.34-3.12 (m, 2H), 2.97-2.90 (m, 2H), 2.41-2.37 (m, 1H), 2.31-2.27 (m, 1H), 2.18-2.06 (m, 2H), 1.67 (s, 3H), 1.66 (s, 3H). ^{31}P NMR (162MHz, $CDCl_3$): δ 115.7.

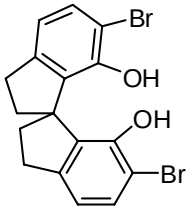
[5] Birman, V. B.; Rheingold, A. L.; Lam, K.-C. *Tetrahedron: Asymmetry*, **1999**, *10*, 125.



(*R*)-**9d**. Synthesized via a modification Puddephat's pocedure from commercially available (*R*)-SHIP.[3] ^{1}H NMR (400MHz, $CDCl_3$): δ 7.41 (t, *J* = 8.0Hz, 2H), 7.33-7.27 (m, 2H), 7.26-7.18 (m, 5H), 7.14 (d, *J* = 8.0Hz, 1H), 6.97 (d, *J* = 8.0Hz, 1H), 3.18-3.09 (m, 2H), 2.97-2.87 (m, 2H), 2.35-2.29 (m, 2H), 2.11-2.04 (m, 2H). ^{31}P NMR (162MHz, $CDCl_3$): δ 108.5.

Synthesis of catalysts **10**:

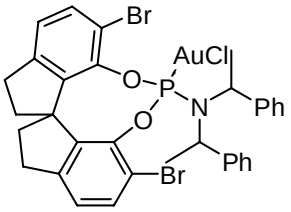




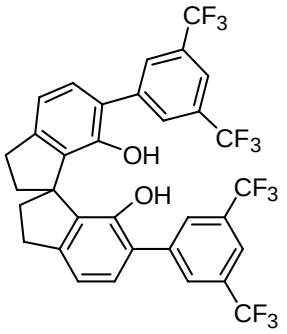
6,6'-dibromo spirobiindane. Obtained through the slow addition of NBS to SPINOL following a patented procedure for the *ortho*-bromination of 4-indanol (73% yield).[6] ^{1}H NMR (400MHz, $CDCl_3$): δ 7.33 (d, *J* = 8.0Hz, 2H), 6.76 (6.76, *J* = 8.0Hz), 5.31 (s, 2H), 3.10-2.96 (m, 4H), 2.45-2.39 (m, 2H),

[6] The *ortho*-bromination of 4-indanol has been recently reported, see: Chhipa, L.; Zambad, S. P.; Gupta, R.; Tuli, D.; Kasundra, A.; Munshi, S.; Siddiqui, M. A.Bhattamisra, S. K.; Dutt, C.; Chauthaiwale, V. Pyrazole derivatives as thyroid receptor modulators and their preparation, pharmaceutical compositions and use in the treatment of diseases. WO 2008149379, July 02, 2008.

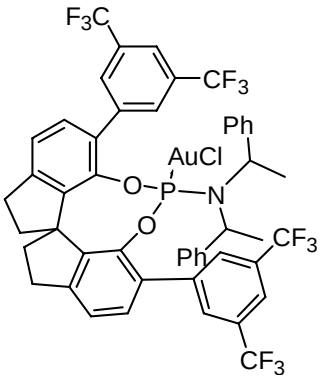
2.28-2.22 (m, 2H). ^{13}C NMR (100MHz, $CDCl_3$): δ 148.5, 145.4, 134.2, 131.0, 118.0, 107.9, 59.7, 38.1, 31.1. The regiochemistry was confirmed from nOe experiments (see spectral data section).



(*R*,*R*,*R*)-**10a**. ^{1}H NMR (400MHz, $CDCl_3$): δ 7.53 (d, *J* = 7.6Hz, 1H), 7.42 (d, *J* = 8.0Hz, 1H), 7.27-7.20 (m, 6H), 7.14-7.12 (m, 4H), 7.04 (d, *J* = 7.6Hz, 1H), 6.99 (d, *J* = 8.0Hz, 1H), 4.48-4.39 (m, 2H), 3.12-2.90 (m, 2H), 2.88-2.77 (m, 2H), 2.34-2.29 (m, 1H), 2.19-2.10 (m, 2H), 1.99-1.91 (m, 1H), 1.86 (s, 3H), 1.84 (s, 3H). ^{31}P NMR (162MHz, $CDCl_3$): δ 116.3.



6,6'-bis(3.5-trifluoromethylphenyl) spirobiindane. Obtained through a variation of the Beller-Köckritz Suzuki protocol in 95%.[7] ^{1}H NMR (500MHz, $CDCl_3$): δ 8.01 (s, 4H), 7.83 (s, 2H), 7.33 (d, *J* = 7.5Hz, 2H), 7.08 (d, *J* = 7.5Hz, 2H), 4.97 (s, 2H), 3.23-3.13 (m, 4H), 2.52-2.48 (m, 2H), 2.43-2.36 (m, 2H). ^{13}C NMR (125MHz, $CDCl_3$): δ 149.8, 147.0, 139.6, 131.6, 131.6, 131.3, 130.6, 129.5, 124.6, 124.5, 122.3, 120.0, 118.6, 57.9, 37.6, 31.1. The regiochemistry was confirmed from nOe experiments (see spectral data section).

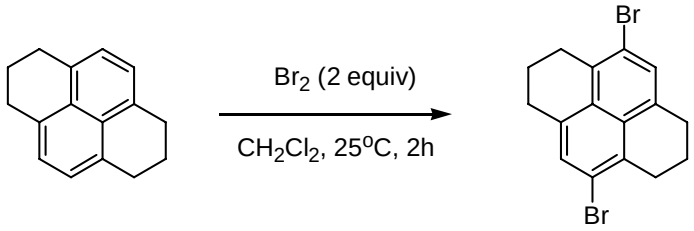


(*R*,*R*,*R*)-**10b**. ^{1}H NMR (400MHz, $CDCl_3$): δ 8.27 (s, 2H), 7.91 (s, 1H), 7.75 (s, 1H), 7.71 (bs, 2H), 7.60 (d, *J* = 7.6Hz, 1H), 7.35 (d, *J* = 7.6Hz, 1H), 7.24 (d, *J* = 7.6Hz, 1H), 7.13 (t, *J* = 7.6Hz, 1H), 7.01 (t, *J* =

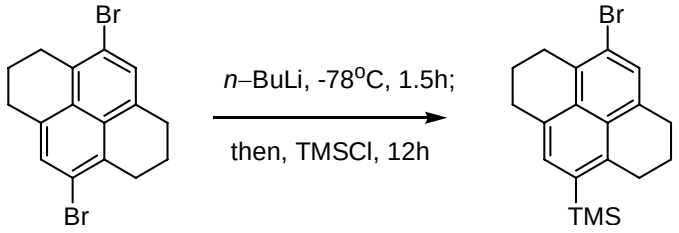
[7] Bartoszek, M.; Beller, M.; Deutsch, J.; Klawonn, M.; Köckritz, A.; Nemati, N.; Pews-Davtyan, A. *Tetrahedron*, **2008**, *64*, 1316.

6.8Hz, 5H), 6.76 (d, J = 6.4Hz, 4H), 4.29-4.19 (m, 2H), 3.32-3.09 (m, 4H), 2.58-2.53 (m, 1H), 2.50-2.42 (m, 1H), 2.33-2.28 (m, 1H), 2.19-2.08 (m, 1H), 0.97 (s, 3H), 0.95 (s, 3H). ^{31}P NMR (162MHz, $CDCl_3$): δ 118.2. HRMS calcd. For $C_{49}H_{36}AuClF_{12}NO_2PNa$ [M + Na] (EI) 1184.1544, found 1184.1525.

Catalyst **11c** was synthesized as follows:

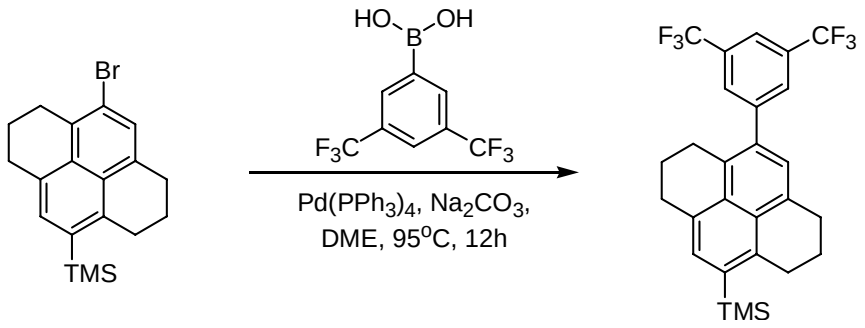


A solution of 1,2,3,6,7,8-hexahydropyrene (19.2mmols, 4g) in dichloromethane (75mL) was placed in a 250mL round bottom flask equipped with a dropping funnel with pressure equalizing arm. Charged in the dropping funnel, a solution of bromide (38.8mmols, 2mL) in dichloromethane (10mL) was added dropwise during a period of 1h. After this period the formed precipitate is filtered, washed with hexanes and dried under vacuum to yield 5.6g (79%) of the desired 4,9-dibromo-H_6-pyrene product as a yellowish powder. ^{1}H NMR (300MHz, $CDCl_3$): δ 7.39 (s, 2H), 3.09-2.96 (m. 8H), 2.06-1.97 (m, 4H). ^{13}C NMR (75MHz, $CDCl_3$): δ 162.3, 135.5, 133.0, 130.6, 128.4, 120.6, 31.3, 30.9, 22.6. HRMS (EI+) calculated for $C_{16}H_{14}Br_2$ 363.9462, found 363.9468.

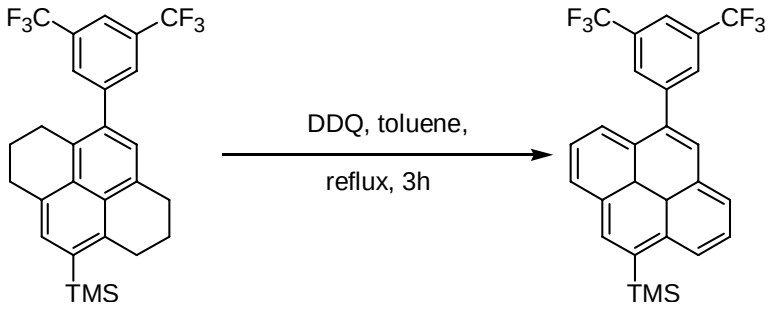


In an oven-dried, cooled under nitrogen, round-bottomed flask 4,9-dibromo-1,2,3,6,7,8-hexahydropyrene (9.0mmols, 3.3g) was weighted in and diluted in dry ether (45mL). At –78°C, n-BuLi (2.5M in hexanes, 9.5mmols, 3.8mL) was added dropwise. After the addition was complete, the solution was stirred for an additional 1.5h. After this period, chlorotrimethylsilane (10.8mmols, 1.37mL) was added and the reaction mixture was allowed to reach room temperature (25°C) and stirred for an additional 12h. The crude reaction mixture was washed with water and ether (3 × 20mL), the combined organic layers were dried over $MgSO_4$, concentrated under vacuum, and purified via silica gel flash column chromatography (hexanes) to give 2.8g (87%) of the desired silane. ^{1}H NMR (300MHz, $CDCl_3$): δ 7.49 (s, 2H), 3.32 (t. J = 6.0Hz, 2H), 3.20 (t, J = 6.3Hz, 2H), 3.14 (t, J = 6.1Hz, 4H), 2.22-2.11 (m, 4H), 0.56 (s, 9H). ^{13}C NMR (75MHz, $CDCl_3$): δ 141.1, 136.1, 133.3, 132.3, 132.0, 129.6,

128.7, 127.6, 120.7, 32.3, 31.5, 31.3, 31.3, 23.4, 22.8, 0.2. HRMS (EI+) calculated for $C_{19}H_{23}BrSi$ 358.0752, found 358.0756.

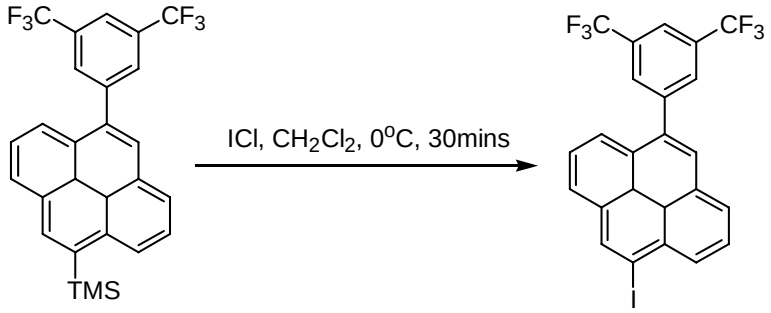


An oven-dried, cooled under nitrogen, three-neck round-bottomed flask equipped with a reflux condenser was charged with 4-bromo-9-trimethylsilyl-1,2,3,6,7,8-hexahydropyrene (6.7mmols, 2.4g), 3,5-bis(trifluoromethyl)phenylboronic acid (11.7mmols, 3.8g), tetrakis(triphenylphosphine)palladium (0.67mmols, 780mg), aq. Na_2CO_3 (2M, 9.1mL) and DME (40mL). The reaction mixture was stirred and heated to reflux for 10h. The crude reaction mixture was cooled to room temperature, passed through a celite pad and the filtrate was concentrated. The concentrated crude was then diluted in dichloromethane (30mL) washed with sat. Ammonium chloride (30mL), water (30mL), then Brine (30mL). The organic layer was dried over $MgSO_4$, filtered and concentrated. The crude mixture was then purified via silica gel flash column chromatography (hexanes) to yield 2.7g (82%) of the desired coupling product. ^{1}H NMR (400MHz, $CDCl_3$): δ 8.03 (s, 1H), 8.00 (s, 2H), 7.53 (s, 1H), 7.23 (s, 1H), 3.37 (t, J = 6.0Hz, 2H), 3.24-3.20 (m, 4H), 3.07 (t, J = 5.9Hz, 2H), 2.25-2.21 (m, 2H), 2.13-2.09 (m, 2H), 0.55 (s, 9H). ^{13}C NMR (100MHz, $CDCl_3$): δ 144.4, 141.0, 135.0, 134.1, 133.5, 133.4, 131.3, 131.0, 130.8, 129.9, 129.7, 129.6, 125.2, 124.9, 122.2, 120.6, 32.6, 31.6 (2C), 29.6, 23.5, 23.2, 0.2. HRMS (EI+) calculated for $C_{27}H_{26}F_6Si$ 492.1708, found 492.1719.

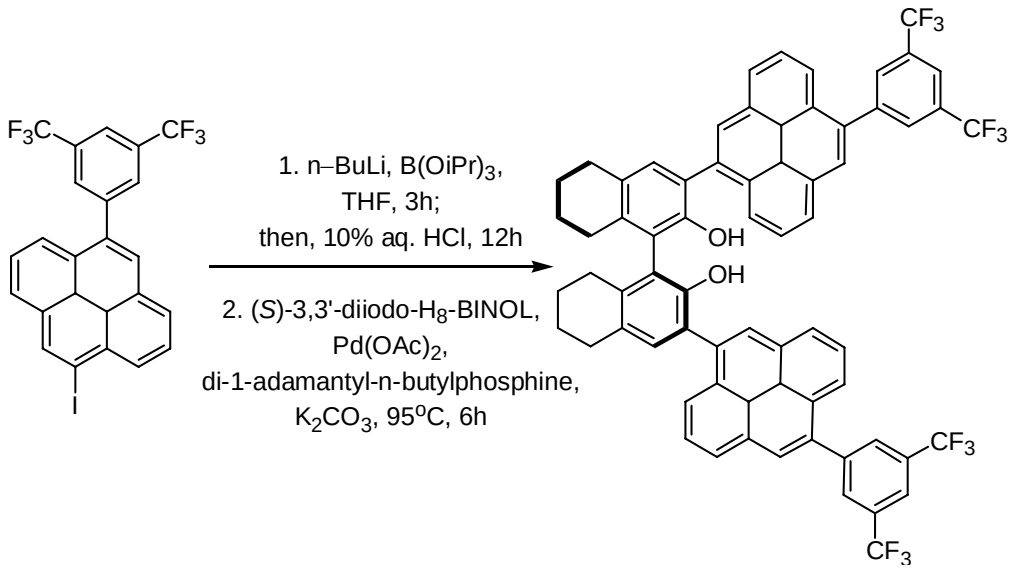


An oven-dried, cooled under nitrogen, round-bottomed flask, equipped with a reflux condenser, was charged with 4-trimethylsilyl-9-(3,5-bistrifluoromethylphenyl)-1,2,3,6,7,8-hexahydropyrene (5.5mmols, 2.7g) and DDQ (16.5mmols, 3.7g) and these were diluted in toluene (25mL). The reaction mixture was then stirred at reflux temperature for 3h. After this period the reaction mixture was cooled to room

temperature and the precipitate was filtered and washed with benzene. The filtrate was concentrated under vacuum, diluted in diethyl ether (30mL) and then washed with a 10% aq. NaOH solution (30mL) and water (30mL). The organic layer was dried over $MgSO_4$, concentrated under vacuum and purified via silica gel flash column chromatography (benzene) to yield 2.3g (86%) of the desired product. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.66 (d, *J* = 7.7 Hz, 1H), 8.50 (s, 1H), 8.33-8.05 (m, 9H), 0.81 (s, 9H). ^{13}C NMR (100MHz, $CDCl_3$): δ 143.1, 137.9, 135.9, 135.9, 134.1, 132.2, 131.9, 130.8, 130.8, 130.3, 129.2, 129.1, 127.5, 127.5, 126.1, 126.0, 125.4, 125.4, 124.9, 124.5, 123.1, 122.7, 121.5. HRMS (EI+) calculated for $C_{27}H_{20}F_6Si$ [M – 2H] 486.1238, found 486.1232.

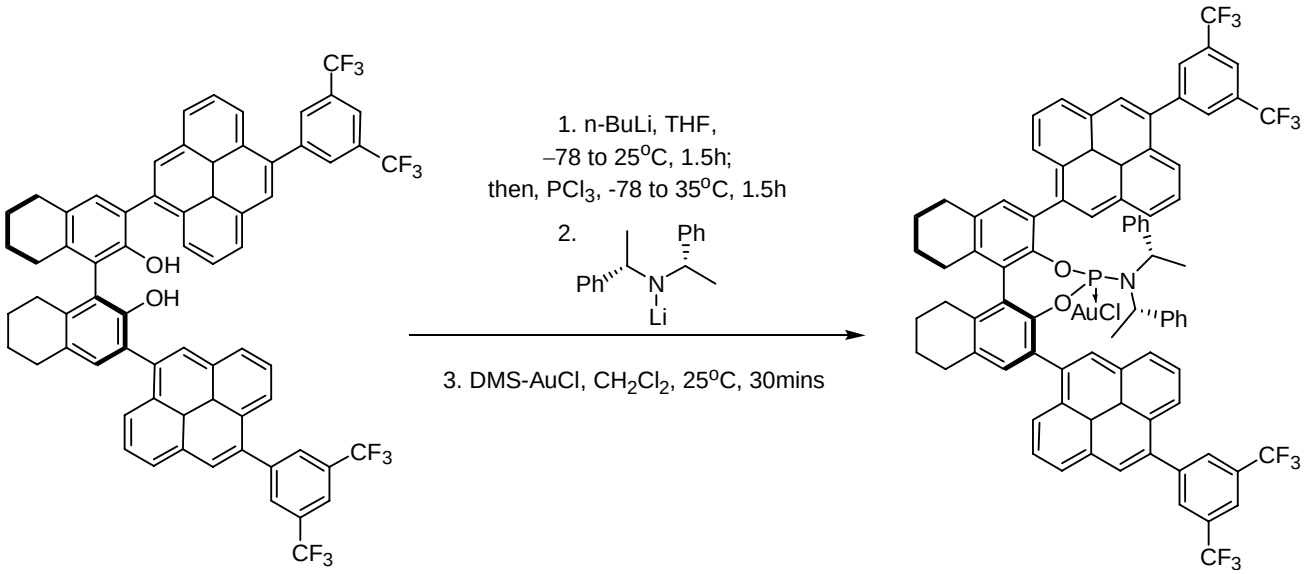


To a solution of 4-trimethylsilyl-9-(3,5-bistrifluoromethylphenyl)-pyrene (3.9mmols, 1.9g) in dichloromethane (130mL) was added ICl (4.7mmols, 0.53mL) dropwise at 0°C. The reaction mixture was allowed to react at this temperature for 30 mins during which period a precipitate was formed. The solid was filtered, washed with dichloromethane and dried under vacuum to yield 2.1g (98%) of 4-iodo-9-(3,5-bistrifluoromethylphenyl)pyrene. ^{1}H NMR (300MHz, $CDCl_3$): δ 8.81 (s, 1H), 8.52 (d, *J* = 7.9Hz, 1H), 8.27 (d, *J* = 7.2Hz, 1H), 8.17-8.10 (m, 4H), 8.05-8.04 (m, 2H), 8.01-7.99 (m, 2H). HRMS (EI+) calculated for $C_{24}H_{12}F_6I$ [M – H] 540.9888, found 540.9838.



A flame-dried round-bottomed flask was charged with the above aryl iodide (3.9mmols, 2.1g) in THF (75mL) and the solution was cooled to −78°C. At this temperature, n-BuLi (2.5M in hexanes, 3.9mL) was added dropwise and the reaction mixture was stirred for 1.5h. After this period, triisopropylborate was added and the mixture was then allowed to warm up to room temperature and stirred for an additional 2h. The crude mixture was poured into 10% aq. HCl and stirred for 12h. The crude was then washed with water and ether (3 × 30mL). The combined organic layers were dried over $MgSO_4$, filtered and the filtrate concentrated under vacuum. The product was then crystallized from hexanes, decanted and dried under vaccum to afford 1.7g (95%) of the desired boronic acid.

An oven-dried, cooled under nitrogen, three-neck round-bottomed flask, equipped with a reflux condenser was charged with 9-(3,5-bistrifluoromethylphenyl)-4-pyrenylboronic acid (3.3mmols, 1.6g), (*S*)-3,3'-diiodo-H_8-BINOL (1.08mmols, 600mg), palladium acetate (0.02mmols, 6mg), di-1-adamantyl-n-butylphosphine (0.03mmols, 12mg), aq. K_2CO_3 (1M, 6.6mL) and DME (12mL). The reaction mixture was stirred and heated to reflux for 6h. The crude reaction mixture was cooled to room temperature, filtered through a celite pad and the filtrate was concentrated. The concentrated crude was then diluted in dichloromethane (30mL) washed with sat. ammonium chloride (30mL), water (30mL), then Brine (30mL). The organic layer was dried over $MgSO_4$, filtered and concentrated. The crude mixture was then purified via silica gel flash column chromatography (9:1 hexanes:EtOAc) to yield 9.3g (77%) of the desired diol. ^{1}H NMR (400MHz, $CDCl_3$): δ 8.30-8.26 (m, 3H), 8.25-8.16 (m, 9H), 8.11-8.01 (m, 9H), 7.97 (t, *J* = 7.6Hz, 1H), 7.91 (t, *J* = 7.6Hz, 1H), 5.01 and 4.95 (s, 1H), 4.90-4.89 (ad, *J* = 3.6Hz, 1H), 2.91 (abs, 4H), 2.67-2.49 (m, 4H), 1.94-1.89 (m, 8H). HRMS calculated for $C_{68}H_{46}F_{12}O_2$ [M − 5H] 1117.2920, found 1117.2912.



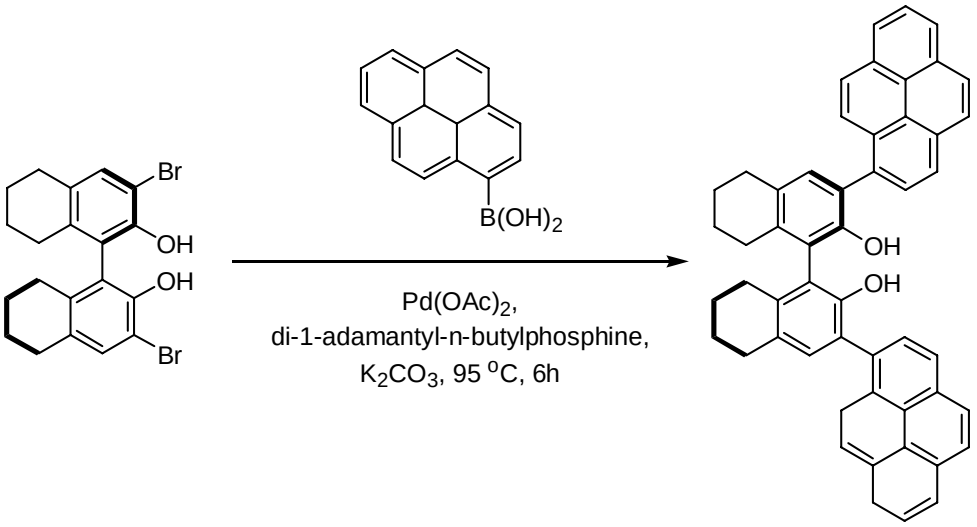
To a solution of the diol (0.53mmols, 600mg) in THF (2.5mL), n-BuLi (2.5M in hexanes, 0.42mL) was added at −78°C and the reaction mixture was allowed to stir at this temperature for 10 mins, then warmed to 25°C and stirred for an additional 90 mins. After this period, the solution was cooled to −78°C and PCl_3 (0.53mmols, 0.046mL) was added. The reaction mixture was stirred at room temperature for another 90 mins.

In parallel, at 0°C, to a solution of (*S*, *S*)-bis(1-phenylethyl)amine (0.53mmols, 0.12mL) in THF (2mL) was added n-BuLi (2.5M in hexanes, 0.21mL) and stirred at this temperature for 30 mins.

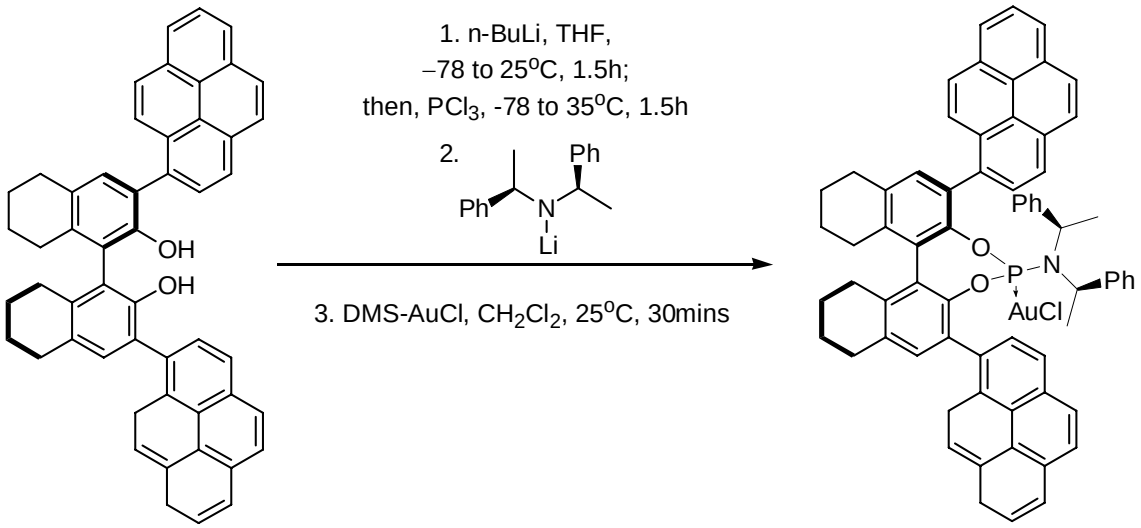
The lithiated amine was then added to the first reaction mixture at −78°C and the reaction mixture was allowed to warm up to room temperature and stirred for 12h. After this period, benzene (10mL) was added to the crude mixture and stirred for 1h. The mixture was then filtered through a silica gel pad and washed with ether. The filtrate was concentrated under vaccum and purified via silica gel column chromatography (98:2 hexanes:EtOAc, Rf = 0.4) to yield the desired phosphoramidite in 64% (436mg).

11c. Au(I) complexes were synthesized via a modification of Puddephat pocedure.[8] To a solution of the phosphoramidite (0.073mmol, 100mg) in dichloromethane (1ml) was added DMS-AuCl (0.073mmols, 22mg) and the mixture was allowed to stir at room temperature for 30 mins. The reaction mixture was concentrated under vaccum and purified via silica gel flash column chromatography (95:5, hexanes:EtOAc, Rf = 0.5) to yield the corresponding gold(I) complex **11c** in 91% (107mg). ^{1}H NMR (400MHz, $CDCl_3$) shows a complex mixture of isomers: δ 8.78-8.77 (m, 1H), 8.61 (ad, *J* = 6.0Hz, 1H), 8.37 (bs, 1H), 8.31-7.57 (m, 21H), 7.51-7.45 (m, 2H), 6.47-6.44 (m, 2H), 5.96-5.84 (m, 6H), 5.60 (d, *J* = 7.2Hz, 2H), 4.23-4.21 (m, 1H), 3.82-3.79 (m, 1H), 3.08-3.02 (m, 6H), 2.73-2.69 (m, 2H), 2.18-1.81 (m, 8H), 0.33-0.20 (m, 6H). ^{31}P NMR (161MHz, $CDCl_3$): δ 126.1, 125.8. See bellow ORTEP of (*S*, *S*, S)-**11c**, ellipsoids are drawn at the 30% probability level:

[8] Brandys, M.-C.; Jennings, M. C.; Puddephat, R. J. *Dalton* **2000**, 4601.



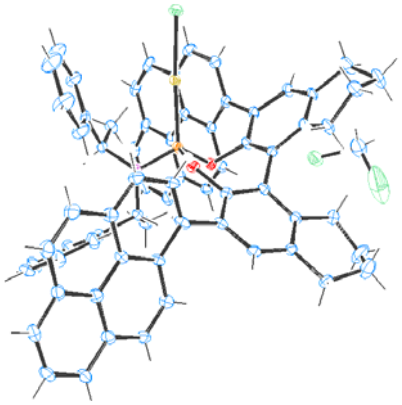
3,3'-di(1-pyrenyl)-5,6,7,8,5',6',7',8'-octahydro-(1,1'-binaphthalene)-2,2'-diol (3,3'-bis(1-pyrenyl)-H_8-BINOL) was synthesized following the Beller-Köckritz procedure from commercially available 1-pyrenylboronic acid and 3,3'-dibromo-5,6,7,8,5',6',7',8'-octahydro-(1,1'-binaphthalene)-2,2'-diol.[9] ^{1}H and ^{13}C NMR anylysis of the products revealed a complex mixture of isomers. ^{1}H NMR (400MHz, $CDCl_3$): δ 8.32-7.35 (m, 19H), 7.36 (ad, J = 5.6Hz, 2H), 5.12-4.99 (m, 2H), 2.99-2.60 (m, 8H), 2.17-1.86 (m, 8H). ^{13}C NMR (100MHz, $CDCl_3$): δ 148.9, 148.8, 137.2, 137.1, 133.0, 131.4 (3C), 131.1, 131.0, 131.0, 130.1, 130.0, 129,3 (3C), 128.5, 128.4, 128.3, 127.7, 127.6 (3C), 127.5 (2C), 127.4, 126.1 (3C), 125.6 (3C), 125.3, 125.2 (2C), 125.1, 125.0, 124.9, 124.8, 121.0, 120.9, 120.8, 34.8, 34.6, 31.8, 29.4, 27.6, 27.5, 25.4, 23.4, 23.3, 23.2, 22.8.

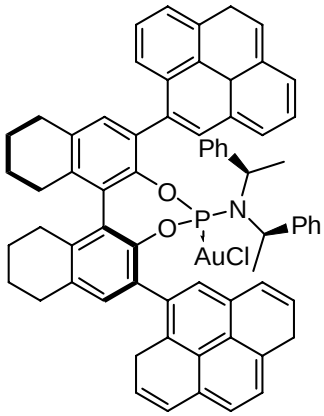


11a. Synthesized following the above mentioned procedure for the synthesis of **11c**. ^{1}H NMR (400MHz, $CDCl_3$): δ 8.56-8.54 (m, 1H), 8.43-8.41 (m, 1H), 8.29-7.93 (m, 19H), 7.74-7.39 (m, 1H), 6.41-6.39 (m, 1H), 6.23-6.21 (m, 1H), 6.04-5.97 (m, 4H), 5.84-5.27 (m, 4H), 4.09-3.97 (m, 1H), 3.87-

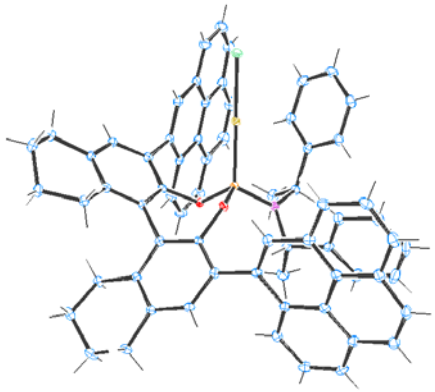
[9] Bartoszek, M.; Beller, M.; Deutsch, J.; Klawonn, M.; Köckritz, A.; Nemati, N.; Pews-Davtyan, A. *Tetrahedron*, **2008**, *64*, 1316.

3.72 (m, 1H), 3.15-2.89 (m, 6H), 2.74-2.56 (m, 2H), 2.13-1.87 (m, 8H), 0.34-0.24 (m, 6H). ^{31}P NMR (162MHz, $CDCl_3$): δ 125.9, 125.0. HRMS (ESI) calculated for $C_{68}H_{54}O_2NAuP$ [M – HCl] 1144.3552, found 1144.3536. See bellow ORTEP of (*R*, *R*, *R*)-**11a**, ellipsoids are drawn at the 30% probability level:



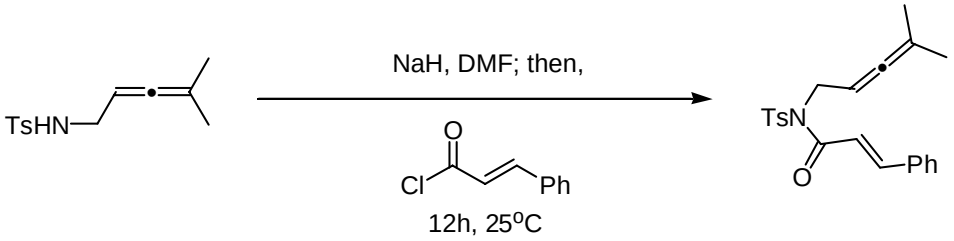


11b. Synthesized following the above mentioned procedure for the synthesis of **11c**. ^{1}H NMR (400MHz, $CDCl_3$): δ 8.78-8.71 (m, 1H), 8.53-8.51 (m, 1H), 8.31-7.93 (m, 15H), 7.83-7.41 (m, 3H), 6.39-6.37 (m, 2H), 5.86-5.75 (m, 6H), 5.55-5.53 (d, *J* = 8.0Hz, 2H), 4.19-4.12 (m, 1H), 3.79-3.73 (m, 1H), 3.04-2.96 (m, 6H), 2.88-2.59 (m, 2H), 2.03-1.94 (m, 8H), 0.28-0.14 (m, 6H). ^{31}P NMR (162MHz, $CDCl_3$): δ 125.9, 125.7. HRMS (FAB+) calculated for $C_{68}H_{54}O_2NAuClP$ [M – 2H] 1179.3241, found 1179.3263. See bellow ORTEP of (*S*, *S*, *S*)-**11b**, ellipsoids are drawn at the 30% probability level:

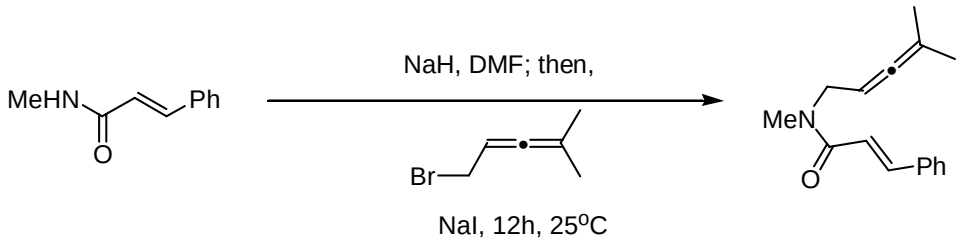


2.3 Preparation and Characterization of Substrates

Substrates **1** were synthesized following a published literature procedure.[10] For a couple of representative procedures see bellow:



12, Prepared by a modification of a procedure reported by Tanaka.[11] To a suspension of NaH (95%, 2.9mmols, 68mg) in DMF (6mL) the sulfonamide[12] (2.4mmols, 600mg) was added dropwise at 0°C and allowed to react for 10 mins. To this mixture, cinnamoyl chloride (3.6mmols, 601mg) was added and the reaction mixture was allowed to stir for 12h. The crude mixture was partitioned between water and diethyl ether. The combined organic layers were dried over $MgSO_4$, filtered and concentrated under vaccum. The residue was chromatrographed on silica gel eluting with hexanes:EtOAc (85:15, Rf = 0.31) to yield the desired substrate in 85% (780mg). ^{1}H NMR (300MHz, $CDCl_3$): δ 7.87 (d, *J* = 8.4Hz, 2H), 7.67 (d, *J* = 15.3Hz, 1H), 7.49-7.46 (m, 2H), 7.38-7.36 (m, 3H), 7.30 (d, *J* = 8.1Hz, 2H), 7.04 (d, *J* = 15.6Hz, 1H), 5.20-5.15 (m, 1H), 4.52 (d, *J* = 5.4Hz, 2H), 2.4 (s, 3H), 1.64 (s, 3H), 1.63 (s, 3H). ^{13}C NMR (75MHz, $CDCl_3$): δ 202.4, 165.8, 145.7, 144.5, 137.1, 134.4, 130.5, 129.5, 128.9, 128.2, 128.0, 117.8, 99.4, 86.1, 45.6, 21.6, 20.2. HRMS (ESI) calculated for $C_{20}H_{22}O_2N_4S$ [M + H] 382.1458, found 382.1466.



14. To a suspension of NaH (95%, 7.5mmols, 182mg) in DMF (32mL), (*E*)-*N*-methyl-3-phenyl-2-propenamide[13] (6.2mmols, 1g) was added dropwise at 0°C and allowed to react for 10 mins. To this mixture, 1-bromo-2,3-pentadiene[14] (8.2mmols, 1.32g) was added and the reaction mixture was allowed to stir for 12h. The crude mixture was partitioned between water and diethyl ether. The combined

[10] Luzung, M. R.; Mauleón, P.; Toste, F. *J. Am. Chem. Soc.* **2007**, *129*, 12402.
[11] Ohno, H.; Mizutani, T.; Kadoh, Y.; Aso, A.; Miyamura, K.; Fujii, N.; Tanaka, T. *J. Org. Chem.* **2007**, *72*, 4378.
[12] Wender, P. A.; Correa, A. G.; Sato, Y.; Sun, R. *J. Am. Chem. Soc*. **2000**, *122*, 7815.
[13] Schauer, D. J.; Helquist, P. *Synthesis*, **2006**, *21*, 3654.
[14] (a) Wender, P. A.; Glorius, F.; Husfeld, C. O.; Langkopf, E.; Love, J. A. *J. Am. Chem. Soc.* **1999**, *121*, 5348. (b) Murakami, M.; Kadowaki, S.; Matsuda, T. *Org. Lett*. **2005**, *7*, 3953.

organic layers were dried over $MgSO_4$, filtered and concentrated under vaccum. The residue was chromatrographed on silica gel eluting with hexanes:EtOAc (70:30, Rf = 0.26) to yield the desired substrate in 62% (926mg). ^{1}H NMR (300MHz, $CDCl_3$): δ 7.65 (d, *J* = 15.6Hz, 1H), 7.51 (bs, 2H), 7.34 (bs, 3H), 6.89-6.80 (m, 1H), 5.00 (bs, 1H), 4.04-3.97 (m, 2H), 3.03 (s, 3H), 1.64 (bs, 6H). ^{13}C NMR (75MHz, $CDCl_3$): δ 203.2, 143.0, 137.7, 137.1, 132.9, 129.6, 128.8, 128.7, 128.5, 128.1, 127.0, 126.5, 96.3, 83.6, 54.6, 46.2, 27.8, 22.1. HRMS (ESI) calculated for $C_{16}H_{20}NO$ [M + H] 242.1539, found 242.1536.

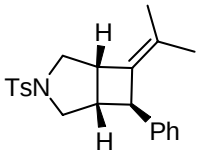
2.4. Au(I)-catalyzed [2+2]-cycloadditions of allenenes.

Representative procedure for Au(I)-catalyzed [2+2]-cycloadditions of allenenes:

Unless otherwise noted most reactions were carried at 25°C. To a small vial was added $AgBF_4$ (5 mol %) and the appropriate catalyst (6 mol %) in dicloromethane (or chloroform when specified) (0.5mL) and the resulting mixture was sonicated for 3 mins. The resulting suspension was filtered through glass fiber into a solution of the corresponding allenene (1.0 equiv) in the same solvent (0.3mL). The reaction mixture was stirred for 12h. After this period, the crude mixture was concentrated and the products were purified via silica gel flash column chromatography.

All racemic material where synthesized utilizing 5 mol % Ph_3PAuCl and 5 mol % $AgBF_4$ in dichloromethane, at 25 °C, following the above mentioned procedure.

The relative and absolute stereochemistry of products **2** was assigned from their correlation with the HPLC trace of that reported in the literature.[15]

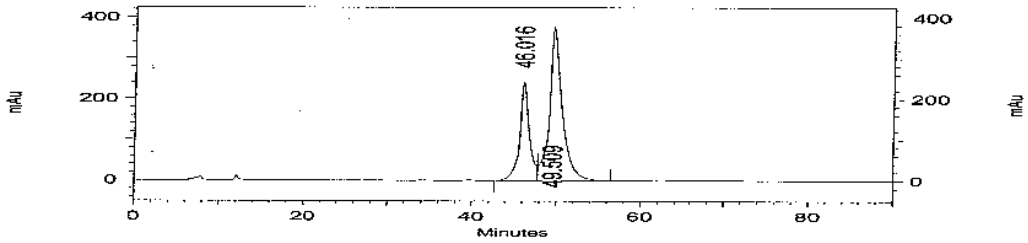


2b For complete characterization see Ref. 10.

HPLC traces for compound **2b**.

[15] Teller, H.; Flugge, S.; Goddard, R.; Fürstner, A. *Angew. Chem., Int. Ed.* **2010**, *49*, 1949.

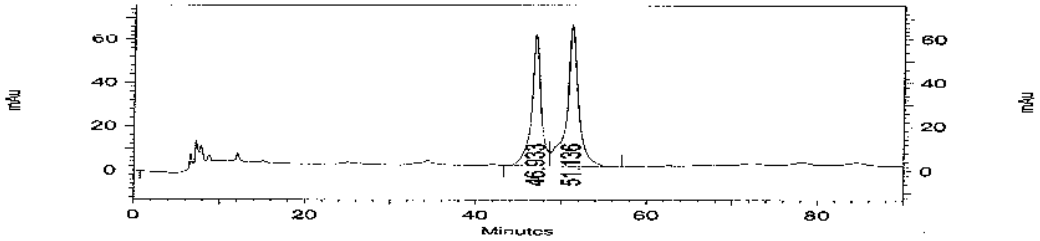
From (*S*,*S*,*S*)-**5a**, Table 1, entry 1, Method:Whelk-O1, hexanes:*i*PrOH, 90:10, 0.5 mL/min:



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
46.016	19286574	32.681
49.509	39727740	67.319

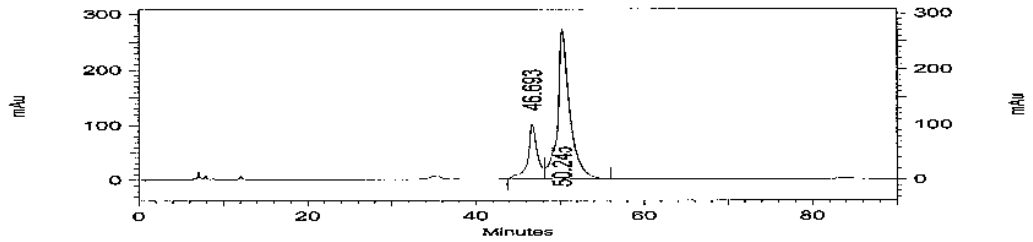
From (*S*,*S*,*S*)-**5b**, Table 1, entry 2, Method:Whelk-O1, hexanes:*i*PrOH, 90:10, 0.5 mL/min:



1: 210 nm, 4 nm Results

Retention Time	Area	Area Percent
46.933	4652935	42.920
51.136	6187906	57.080

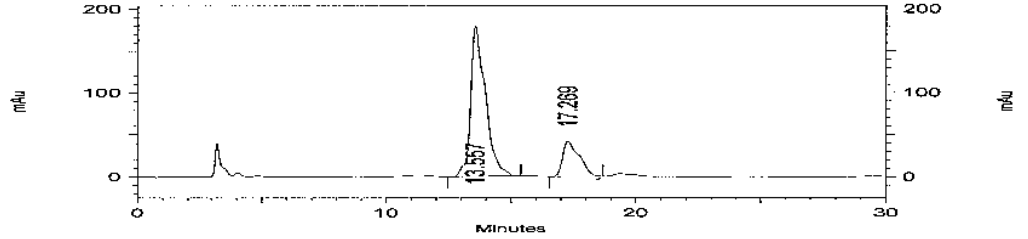
From (*S*,*S*,*S*)-**5c**, Table 1, entry 3, Method:Whelk-O1, hexanes:*i*PrOH, 90:10, 0.5 mL/min:



1: 223 nm, 4 nm Results

Retention Time	Area	Area Percent
46.693	7703609	22.025
50.245	27272655	77.975

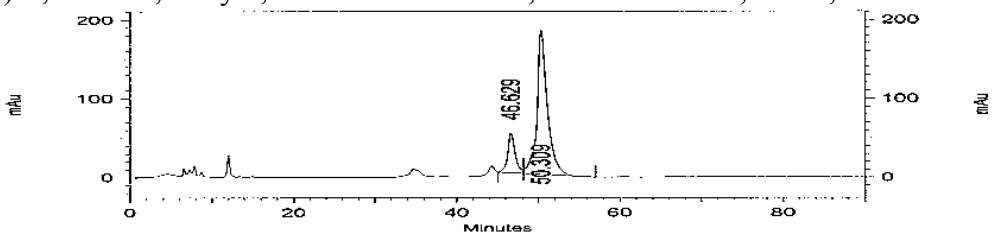
From (*S*,*S*,*S*)-**6**, Table 1, entry 4, Method: Chiracel-AD, hexanes:*i*PrOH, 95:5, 0.5 mL/min:



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
13.557	7389541	79.414
17.269	1915542	20.586

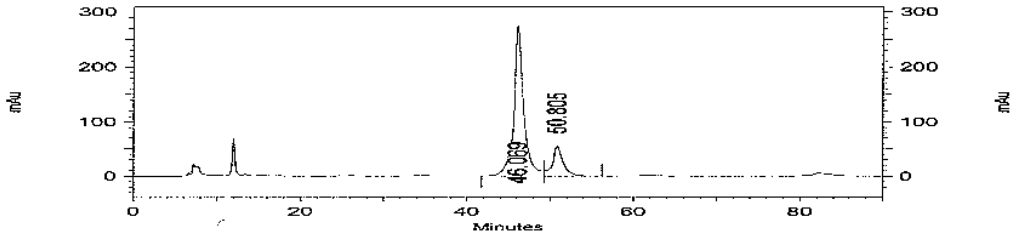
From (*S*,*S*,*S*)-**7**, Table 1, entry 5, Method:Whelk-O1, hexanes:*i*PrOH, 90:10, 0.5 mL/min:



1: 210 nm, 4 nm Results

Retention Time	Area	Area Percent
46.629	3221135	16.570
50.309	16218307	83.430

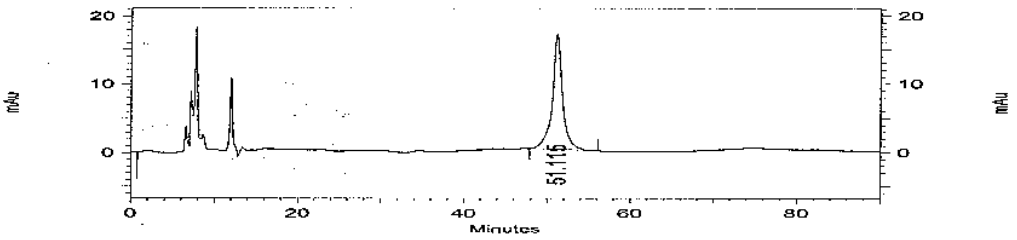
From (*R*,*R*,*R*)-**8**, Table 1, entry 6, Method:Whelk-O1, hexanes:*i*PrOH, 90:10, 0.5 mL/min:



1: 210 nm, 4 nm Results

Retention Time	Area	Area Percent
46.069	22441082	82.472
50.805	4769390	17.528

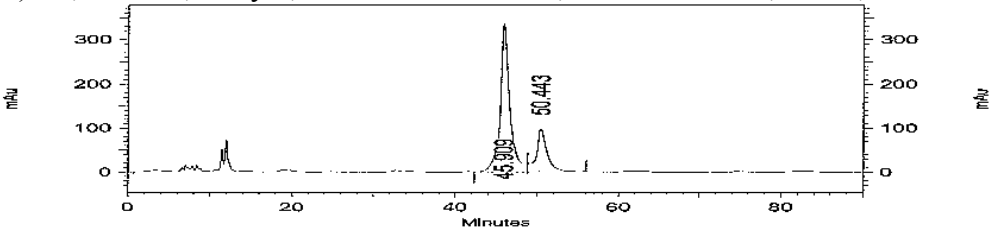
From (*R*,*R*,*R*)-**9a**, Table 1, entry 7, Method:Whelk-O1, hexanes:*i*PrOH, 90:10, 0.5 mL/min, (after crystallization):



1: 210 nm, 4 nm Results

Retention Time	Area	Area Percent
51.115	1428135	100.000

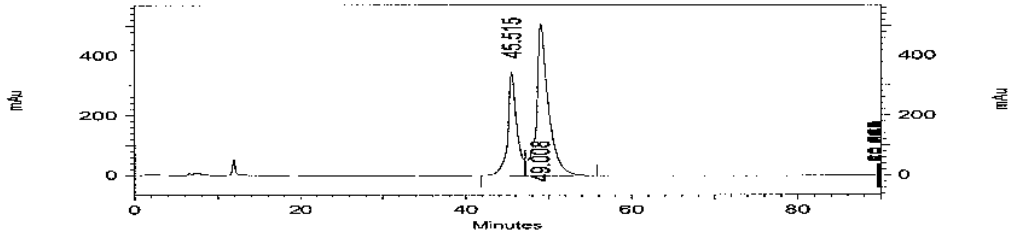
From (*S*,*R*,*R*)-**9a**, Table 1, entry 8, Method:Whelk-O1, hexanes:*i*PrOH, 90:10, 0.5 mL/min:



1: 210 nm, 4 nm Results

Retention Time	Area	Area Percent
45.909	27479728	75.849
50.443	8749674	24.151

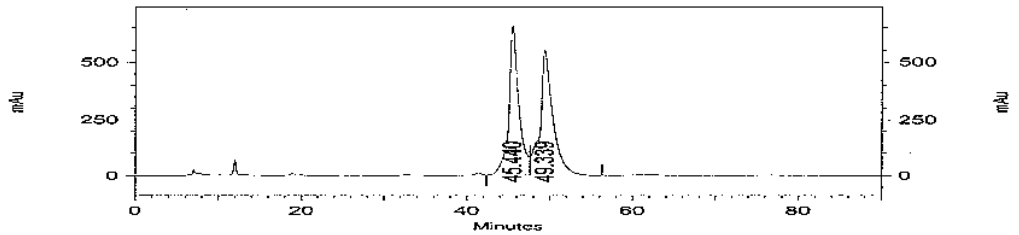
From (*R*,*R*,*R*)-**9b**, Table 1, entry 9, Method:Whelk-O1, hexanes:*i*PrOH, 90:10, 0.5 mL/min:



1: 210 nm, 4 nm Results

Retention Time	Area	Area Percent
45.515	26327435	34.080
49.008	50922901	65.918

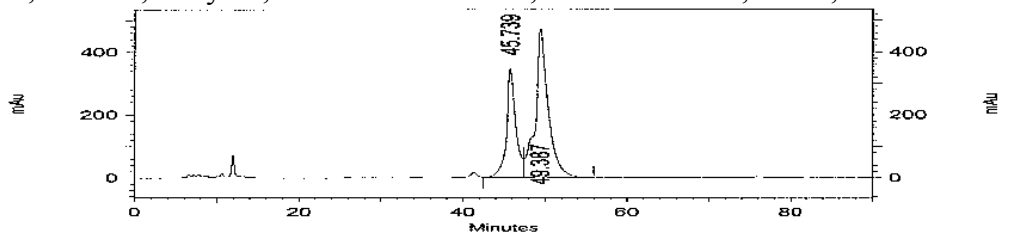
From (*R*,*R*,*R*)-**9c**, Table 1, entry 10, Method:Whelk-O1, hexanes:*i*PrOH, 90:10, 0.5 mL/min:



1: 210 nm, 4 nm Results

Retention Time	Area	Area Percent
45.440	55866314	48.225
49.339	59978761	51.775

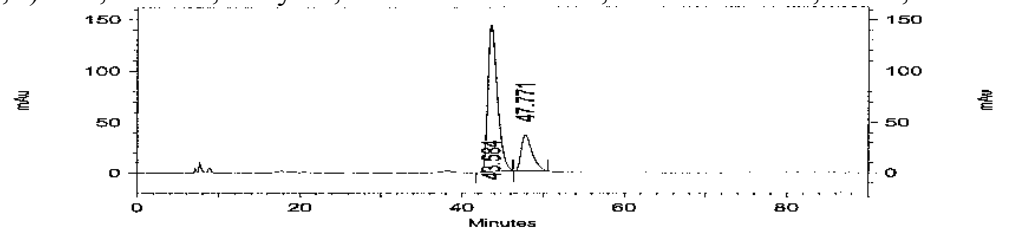
From (*R*)-**9d**, Table 1, entry 11, Method:Whelk-O1, hexanes:*i*PrOH, 90:10, 0.5 mL/min:



1: 210 nm, 4 nm Results

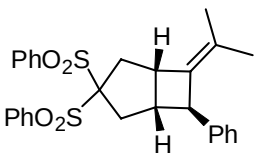
Retention Time	Area	Area Percent
45.739	27006922	34.321
49.387	51681339	65.679

From (*R*,*R*,*R*)-**10a**, Table 1, entry 12, Method:Whelk-O1, hexanes:*i*PrOH, 90:10, 0.5 mL/min:



1: 230 nm, 4 nm Results

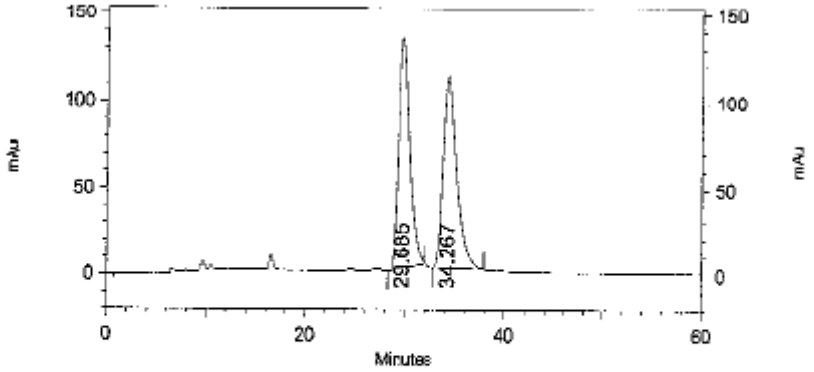
Retention Time	Area	Area Percent
43.584	11699378	77.773
47.771	3343621	22.227



2c Purified via silica gel flash column chromatography (hexanes:EtOAc, 90:10) 82% yield.For complete characterization see Ref. 10.

HPLC traces for compound **2c**.

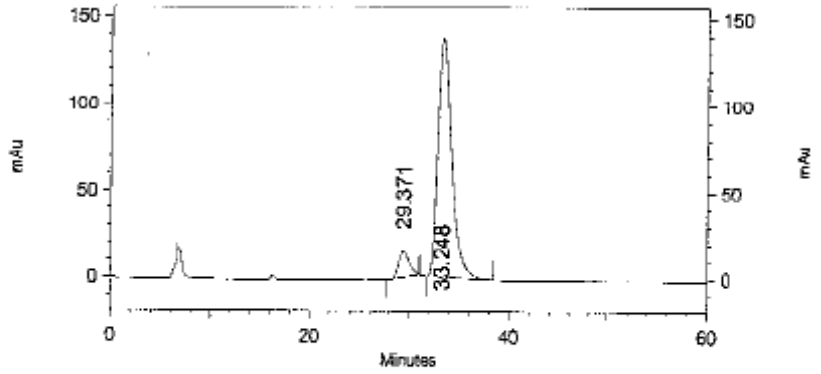
Racemic, Method: Chiracel OD, hexanes:EtOH, 85:15, 0.5 mL/min:



1: 230 nm, 4 nm Results

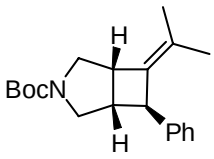
Retention Time	Area	Area Percent
29.685	10389386	49.236
34.267	10711639	50.764

From (*R*,*R*,*R*)-**9a**, Table 2, entry 3, Method: Chiracel OD, hexanes:EtOH, 85:15, 0.5 mL/min:



1: 230 nm, 4 nm Results

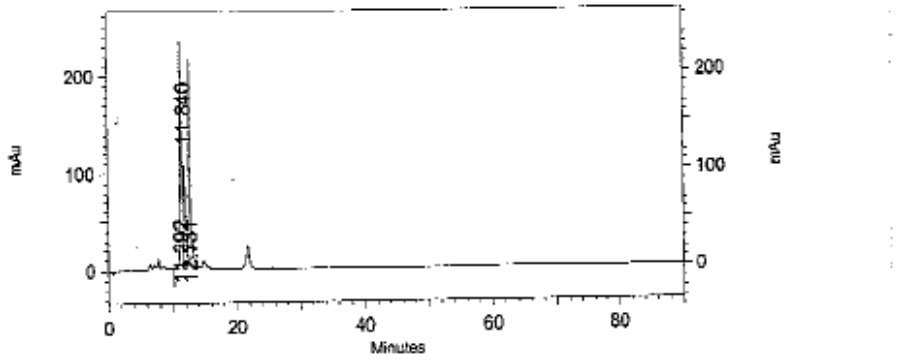
Retention Time	Area	Area Percent
29.371	1121045	7.930
33.248	13014952	92.070



2d. Purified via silica gel flash column chromatography (hexanes:EtOAc, 90:10) 52% yield. ^{1}H NMR (400MHz, $CDCl_3$): δ 7.31-7.25 (m, 3H), 7.20-7.15 (m, 2H), 3.69 (bs, 3H), 3.52 (bs, 1H), 3.26-3.20 (m, 2H), 2.66-2.61 (m, 1H), 2.16 (s, 9H), 1.62 (s, 3H), 1.23 (s, 3H). HRMS calcd. For $C_{20}H_{27}NO_2$ (EI) 313.2042, found 313.2036.

HPLC traces for compound **2d**.

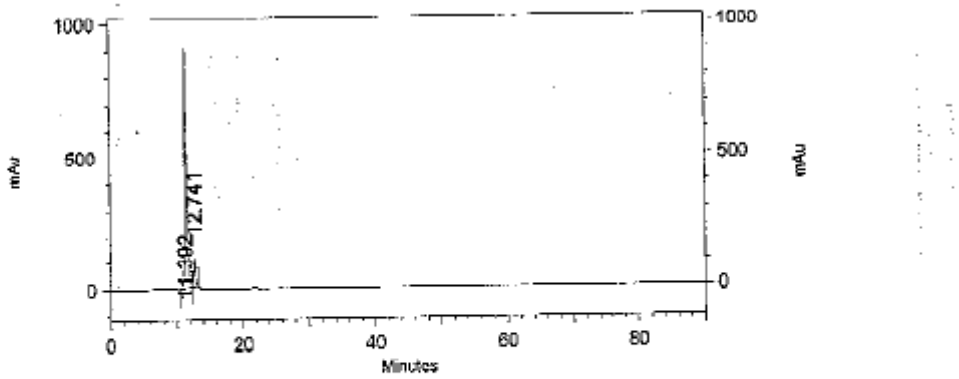
Racemic, Method: Whelk-O1, hexanes:*i*PrOH, 90:10, 0.5 mL/min (minor impurity observable corresponds to catalyst used concluded from it's ^{1}H NMR spectrum):



1: 211 nm, 4 nm Results

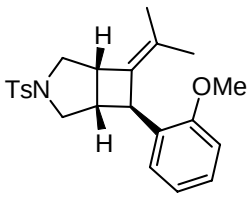
Retention Time	Area	Area Percent
11.392	4010574	41.302
11.840	1792412	18.459
12.731	3907468	40.240

From (*R*,*R*,*R*)-**9a**, Table 2, entry 4, Whelk-O1, hexanes:*i*PrOH, 90:10, 0.5 mL/min:



1: 215 nm, 4 nm Results

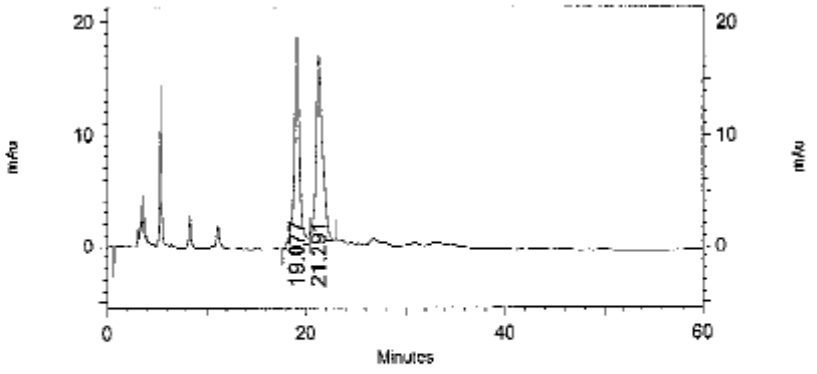
Retention Time	Area	Area Percent
11.392	20030444	90.489
12.741	2105368	9.511



2e. Purified via silica gel flash column chromatography (hexanes:EtOAc, 90:10) 82% yield. ^{1}H NMR (400MHz, $CDCl_3$): δ 7.73, (d, *J* = 8.4Hz, 2H), 7.33 (d, *J* = 8.4Hz, 2H), 7.19 (t, *J* = 6.4Hz, 1H), 7.11 (d, *J* = 7.6Hz, 1H), 6.90-6.83 (m, 2H), 4.09 (bs, 1H), 3.82 (s, 3H), 3.79 (d, *J* = 8.0Hz, 1H), 3.68 (d, *J* = 12.0Hz, 1H), 3.49-3.33 (m, 1H), 2.71-2.63 (m, 2H), 2.44-2.39 (m, 1H), 2.43 (s, 3H), 1.65 (s, 3H), 1.38 (s, 3H). HRMS calcd. For $C_{23}H_{27}NO_3S$ (EI) 397.1712, found 397.1715.

HPLC traces for compound **2e**.

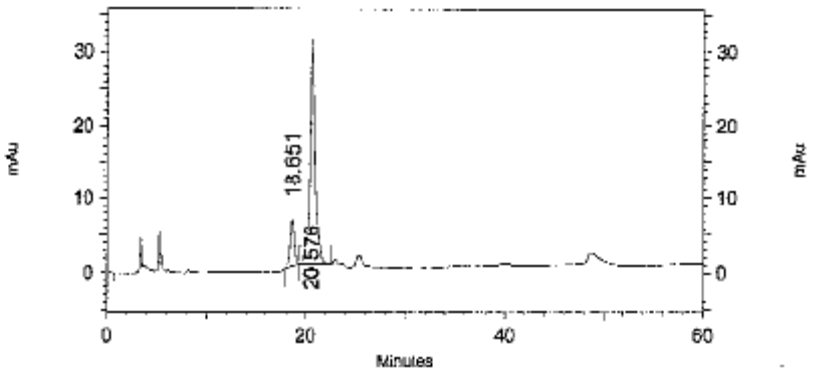
Racemic, Method: Whelk-O1, hexanes:*i*PrOH, 85:15, 1.0 mL/min:



1: 230 nm, 4 nm Results

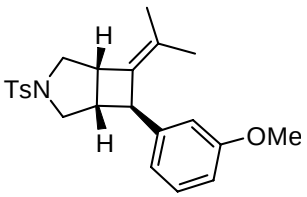
Retention Time	Area	Area Percent
19.077	642017	46.724
21.291	732048	53.276

From (*R*,*R*,*R*)-**9a**, Table 2, entry 5, Whelk-O1, hexanes:*i*PrOH,85:15, 1.0 mL/min:



2: 242 nm, 4 nm Results

Retention Time	Area	Area Percent
18.651	174908	13.069
20.576	1163404	86.931

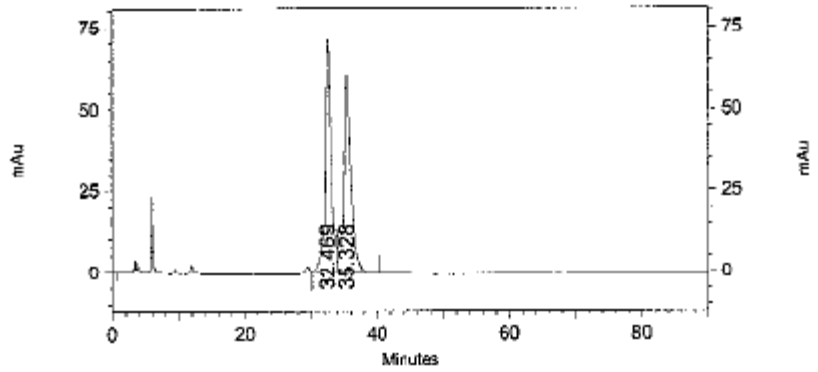


2f. Purified via silica gel flash column chromatography (hexanes:EtOAc, 90:10) 80% yield. ^{1}H NMR (600MHz, $CDCl_3$): δ 7.71 (d, *J* = 8.0Hz, 2H), 7.59-7.41 (m, 1H), 7.31 (d, *J* = 8.0Hz, 2H), 7.21-7.19 (m, 1H), 6.77-6.72 (m, 2H), 3.79 (bs, 4H), 3.69-3.66 (m, 2H), 3.43 (bs, 1H), 2.65-2.51 (m, 3H), 2.44 (s, 3H), 1.60 (s, 3H), 1.30 (s, 3H). ^{13}C NMR (125MHz, $CDCl_3$): δ 159.8, 145.5, 143.6, 132.1, 129.5,

128.8, 128.1, 119.7, 113.1, 111.1, 55.2, 54.0, 53.1, 51.9, 43.9, 42.9, 21.5, 19.1, 18.6. HRMS calcd. For $C_{23}H_{27}NO_3S$ (EI) 397.1712, found 397.1717.

HPLC traces for compound **2f**.

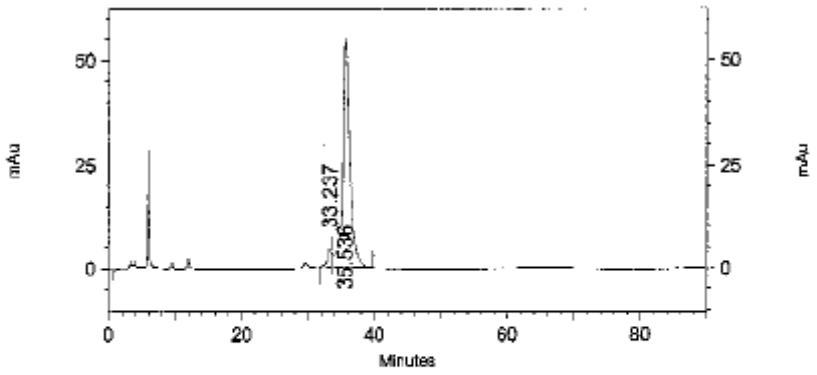
Racemic, Method: Whelk-O1, hexanes:*i*PrOH, 90:10, 1.0 mL/min:



1: 236 nm, 4 nm Results

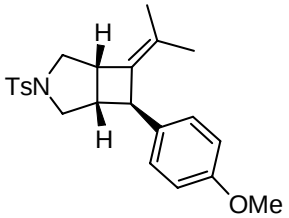
Retention Time	Area	Area Percent
32.469	4412281	49.760
35.328	4454755	50.240

From (*R*,*R*,*R*)-**9a**, Table 2, entry 6, Whelk-O1, hexanes:*i*PrOH, 90:10, 1.0 mL/min:



1: 236 nm, 4 nm Results

Retention Time	Area	Area Percent
33.237	206986	4.870
35.536	4043652	95.130

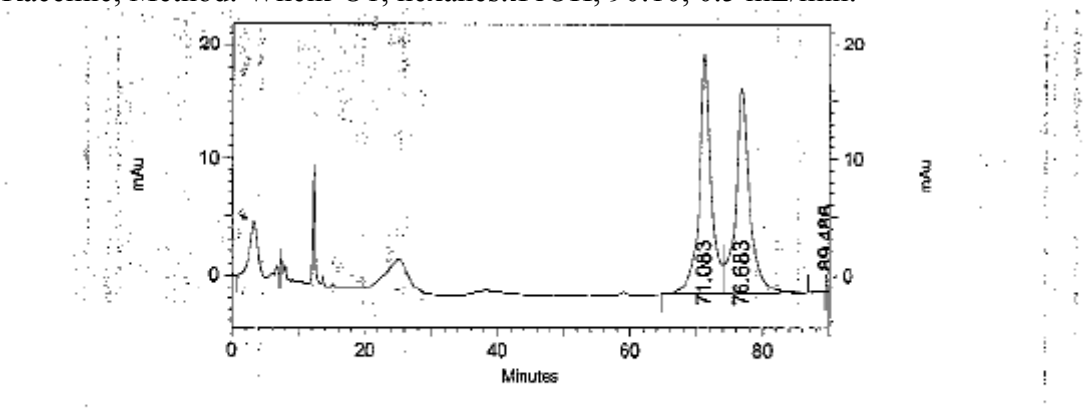


2g. Purified via silica gel flash column chromatography (hexanes:EtOAc, 90:10) 72% yield. ^{1}H NMR (300MHz, $CDCl_3$): δ 7.70 (d, *J* = 8.4Hz, 2H), 7.32 (d, *J* = 8.1Hz, 2H), 7.06 (d, *J* = 8.4Hz, 2H), 6.81 (d,

J = 8.7Hz, 2H), 3.77 (bs, 3H), 3.64 (d, *J* = 9.6Hz, 2H), 3.41 (bs, 1H), 2.68-2.59 (m, 2H), 2.54-2.50 (m, 1H), 2.43 (s, 3H), 1.58 (s, 3H), 1.26 (s, 3H). ^{13}C NMR (125MHz, $CDCl_3$): δ 158.1, 143.6, 135.9, 134.2, 134.1, 132.8, 132.0, 129.5, 129.3, 129.2, 128.3, 128.1, 128.1, 113.9, 55.2, 23.9, 52.9, 51.2, 44.0, 42.8, 21.5, 18.9, 18.7. HRMS calcd. For $C_{23}H_{27}NO_3S$ (EI) 397.1712, found 397.1714.

HPLC traces for compound **2g**.

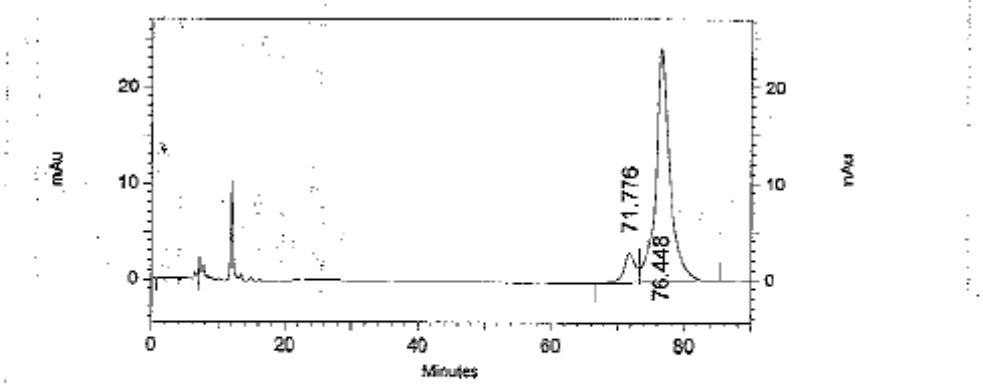
Racemic, Method: Whelk-O1, hexanes:*i*PrOH, 90:10, 0.5 mL/min:



1: 237 nm, 4 nm Results

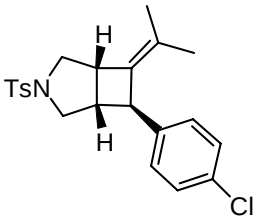
Retention Time	Area	Area Percent
71.083	2591382	49.787
76.683	2613369	50.210

From (*R*,*R*,*R*)-**9a**, Table 2, entry 7, Whelk-O1, hexanes:*i*PrOH, 90:10, 0.5 mL/min:



1: 237 nm, 4 nm Results

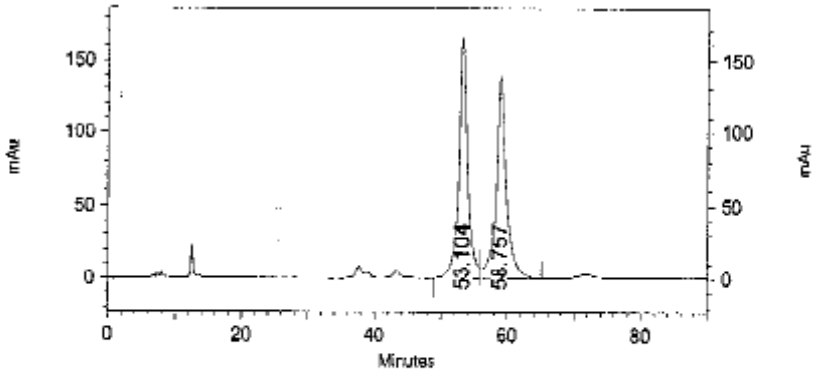
Retention Time	Area	Area Percent
71.776	403915	10.120
76.448	3587426	89.880



2h. Purified via silica gel flash column chromatography (hexanes:EtOAc, 90:10) 87% yield. ^{1}H NMR (600MHz, $CDCl_3$): δ 7.71 (d, *J* = 8.4 Hz, 2H), 7.33 (d, *J* = 8.4Hz, 2H), 7.24 (d, *J* = 7.8Hz, 2H), 7.09 (d, *J* = 8.4Hz, 2H), 3.79 (bs 1H), 3.65 (d, *J* = 9.6Hz, 2H), 3.42 (bs, 1H), 2.67-2.62 (m, 2H), 2.53-2.49 (m, 1H), 2.44 (s, 3H), 1.60 (s, 3H), 1.26 (s, 3H). ^{13}C NMR (150MHZ, $CDCl_3$): δ 143.6, 142.2, 131.9, 131.9, 131.9, 129.5, 129.0, 128.7, 128.5, 128.1, 53.8, 53.0, 51.2, 43.8, 42.8, 21.5, 18.9, 18.7. HRMS calcd. For $C_{22}H_{24}ClNO_2S$ (EI) 401.1216, found 401.1223.

HPLC traces for compound **2h**.

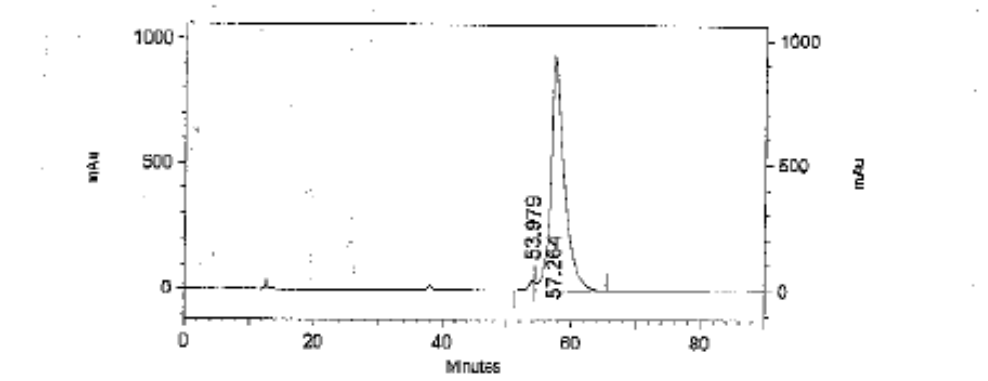
Racemic, Method: Whelk-O1, hexanes:*i*PrOH, 90:10, 0.5 mL/min:



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
53.104	14802045	49.688
58.757	14987946	50.312

From (*R*,*R*,*R*)-**9a**, Table 2, entry 7, Whelk-O1, hexanes:*i*PrOH, 90:10, 0.5 mL/min:



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
53.979	2271870	1.645
57.264	135821446	98.355

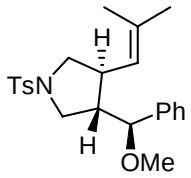
2.5. Au(I)-catalyzed cyclization/alkoxylation of allenenes.

Representative procedure for Au(I)-catalyzed cyclization/alkoxylations of allenenes:

Unless otherwise noted most reactions were carried at 25°C. To a small vial was added $AgBF_4$[16] (5 mol %) and **11c** (6 mol %) in nitromethane (0.5mL) and the resulting mixture was sonicated for 3 mins. The resulting suspension was filtered through glass fiber into a solution of the corresponding allenene (1.0 equiv) and nucleophile (9 equiv) in nitromethane (0.3mL). The reaction mixture was stirred for 12h. After this period, the crude mixture was concentrated and the products were purified via silica gel flash column chromatography.

All racemic material where synthesized utilizing 5 mol % Ph_3PAuCl and 5 mol % $AgBF_4$ in nitromethane, at 25 °C, following the above mentioned procedure.

The relative and absolute stereochemistry of products **3** was assigned from their correlation with the solid state structure of **13b** (see ahead).



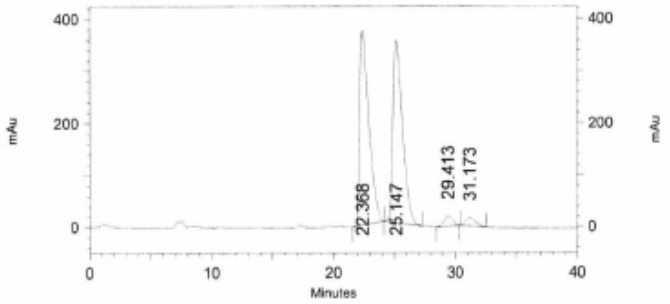
2a. Isolated via silica gel column chromatography (hexanes:EtOAc, 90:10, Rf = 0.2) as a clear oil. ^{1}H NMR (400MHz, $CDCl_3$): δ 7.69 (d, *J* = 8.0Hz, 2H), 7.33-7.24 (m, 5H), 7.14 (d, *J* = 7.6Hz, 2H), 4.57 (d,

[16] When noted $AgSbF_6$ was used instead.

J = 8.8Hz, 1H), 3.86 (d, *J* = 5.7Hz, 1H), 3.46 (t, *J* = 8.3Hz, 2H), 3.22 (t, *J* = 8.2Hz, 1H), 3.12 (s, 3H), 2.80 (dt, *J* = 7.9, 16.5Hz, 1H), 2.72 (t, *J* = 9.1Hz, 1H), 2.44 (s, 3H), 1.95 (dt, *J* = 8.0Hz, 1H), 2.44 (s, 3H), 1.95 (dt, *J* = 8.0Hz, 1H), 1.51 (s, 3H), 1.39 (s, 3H). ^{13}C NMR (125MHz, $CDCl_3$): δ 143.4, 141.2, 134.8, 129.5, 128.4, 127.8, 127.6, 126.7, 123.5, 82.7, 56.8, 53.1, 52.0, 48.9, 39.5, 25.5, 21.5, 17.8. HRMS (EI+): calculated for $C_{23}H_{29}NO_3S$ 399.1868, found 399.1880.

HPLC traces for compound **3a**.

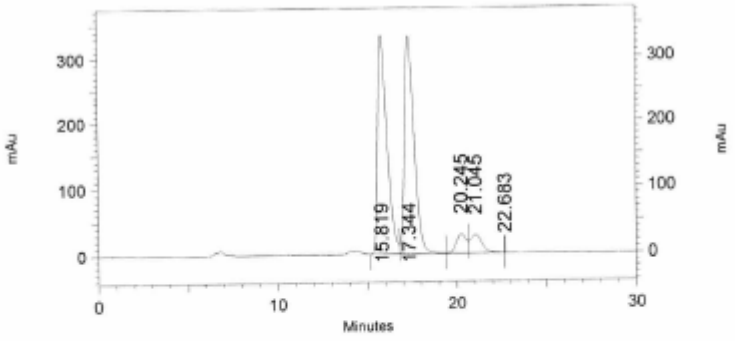
Racemic (minor impurity corresponds to [2+2]-cycloadduct), Method: Chiracel OD, hexanes:*i*PrOH, 93:7, 0.5 mL/min:



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
22.368	19637425	47.914
25.147	19494883	47.567
29.413	944007	2.303
31.173	908159	2.216

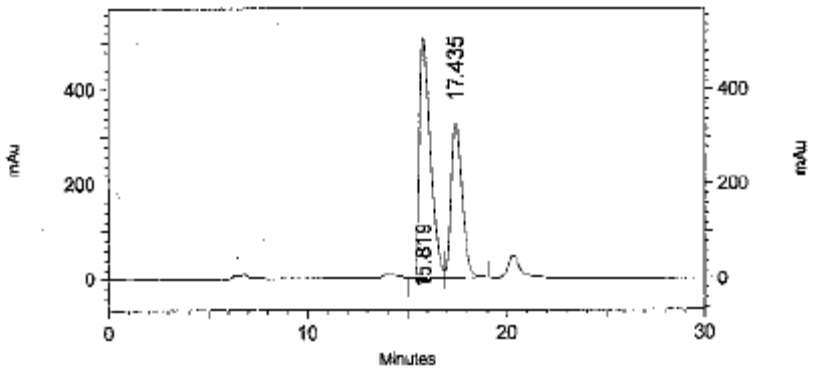
Racemic (minor impurity corresponds to [2+2]-cycloadduct), Method: Chiracel OD, hexanes:*i*PrOH, 88:12, 0.5 mL/min:



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
15.819	12118059	45.013
17.344	12484101	46.373
20.245	1086851	4.037
21.045	1232311	4.577
22.683	14	0.000

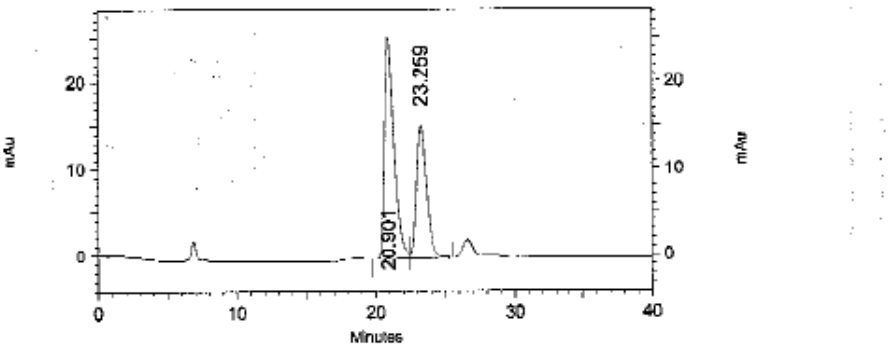
From (*R*,*R*,*R*)-**9a**, Table 3, entry 1**:**



1: 231 nm, 4 nm Results

Retention Time	Area	Area Percent
15.819	19044236	60.321
17.435	12527442	39.679

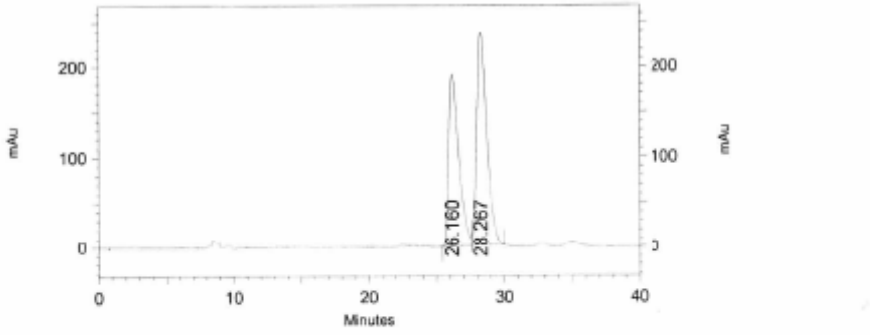
From (*R*,*R*,*R*)-**9a**, Table 3, entry 2**:**



1: 249 nm, 4 nm Results

Retention Time	Area	Area Percent
20.901	1255479	62.045
23.259	768033	37.955

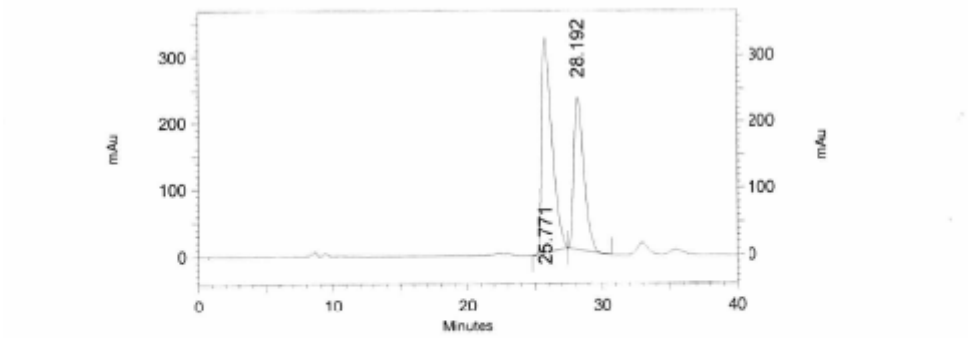
From (*R*,*S*,*S*)-**5a**, Table 3, entry 3**:**



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
26.160	10128956	44.943
28.267	12408368	55.057

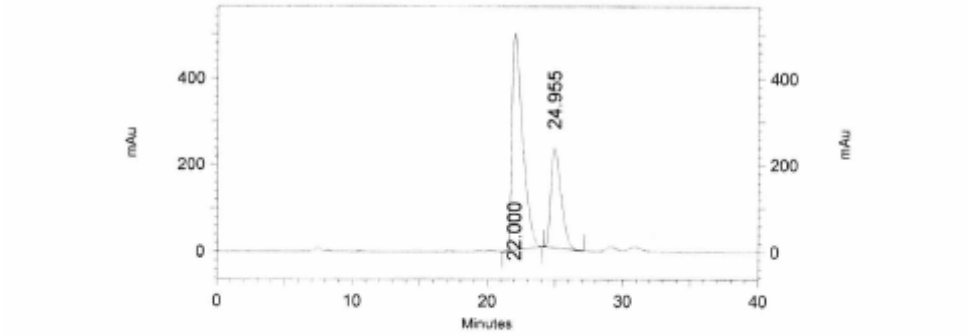
From (*S*,*S*,*S*)-**5a**, Table 3, entry 4**:**



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
25.771	17183175	59.245
28.192	11820451	40.755

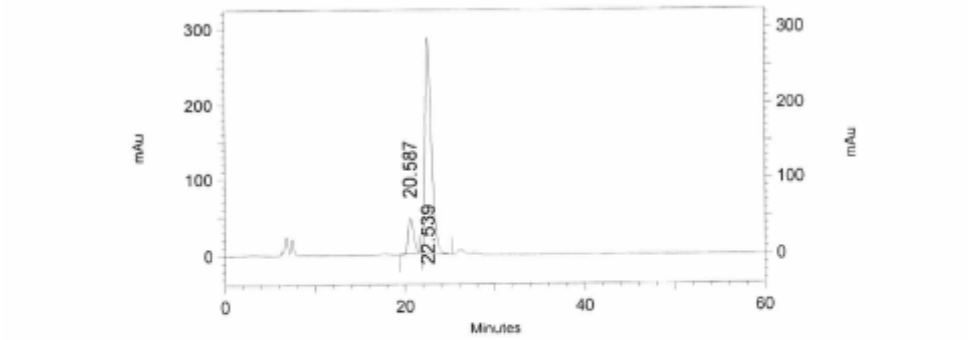
From (*R*,*R*,*R*)-**5b**, Table 3, entry 5**:**



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
22.000	26794879	68.980
24.955	12049378	31.020

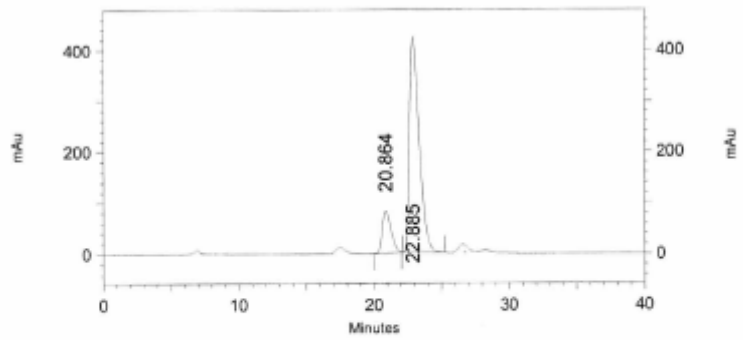
From (*S*,*S*,*S*)-**5c**, Table 3, entry 6**:**



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
20.587	1920738	12.326
22.539	13662067	87.674

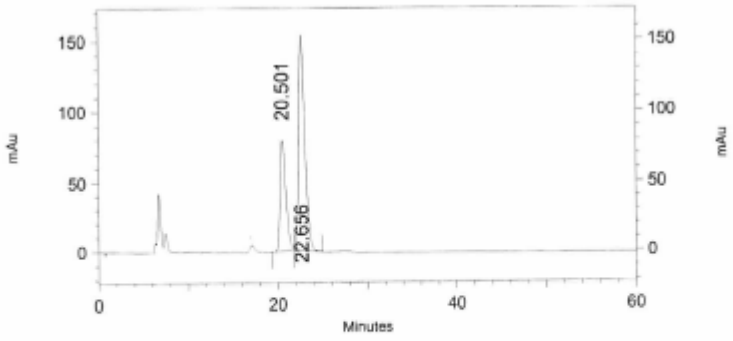
From (*S*,*S*,*S*)-**5c**, Table 3, entry 7**:**



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
20.864	3764250	14.979
22.885	21366048	85.021

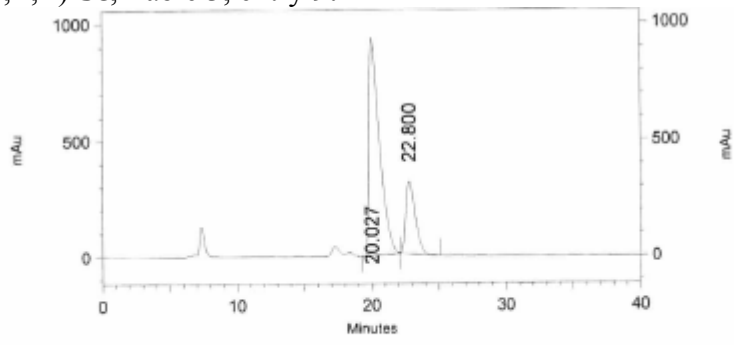
From (*S*,*S*,*S*)-**5d**, Table 3, entry 8**:**



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
20.501	3600963	32.930
22.656	7334375	67.070

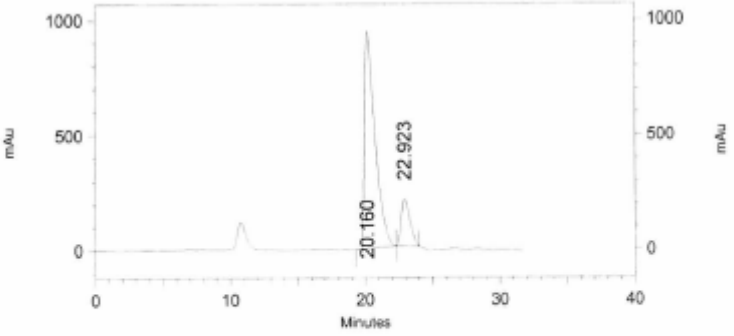
From (*R*,*R*,*R*)-**5e**, Table 3, entry 9**:**



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
20.027	50517867	76.761
22.800	15293778	23.239

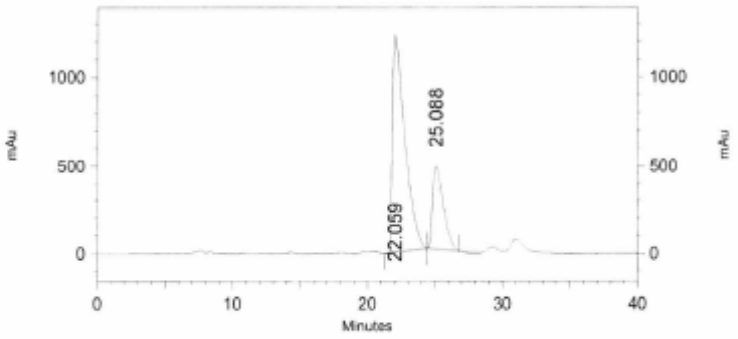
From (*R*,*R*,*R*)-**5e**, Table 3, entry 10 (reaction run at –15°C)**:**



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
20.160	51472154	84.659
22.923	9327068	15.341

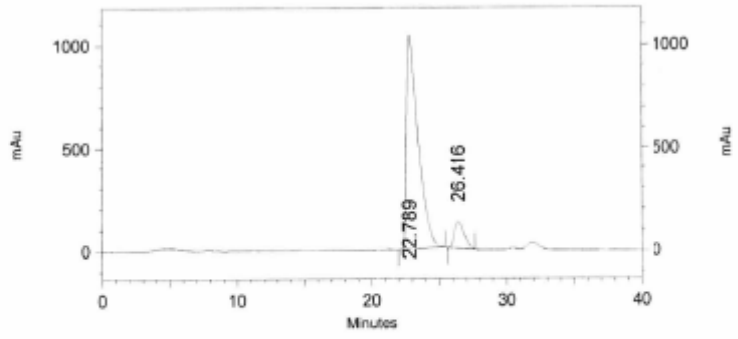
From (*R*,*R*,*R*)-**5f**, Table 3, entry 11**:**



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
22.059	77934092	74.587
25.088	26552899	25.413

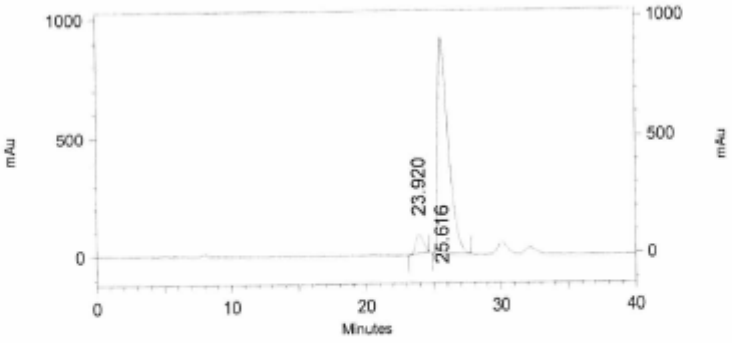
From (*R*,*R*,*R*)-**11a**, Table 3, entry 12**:**



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
22.789	62879846	90.784
26.416	6383127	9.216

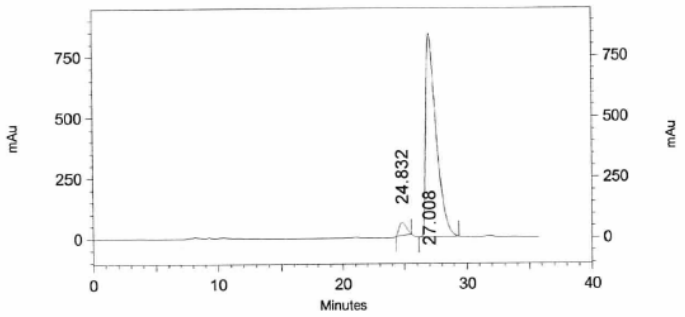
From (*S*,*S*,*S*)-**11b**, Table 3, entry 13**:**



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
23.920	3183510	6.026
25.616	49643765	93.974

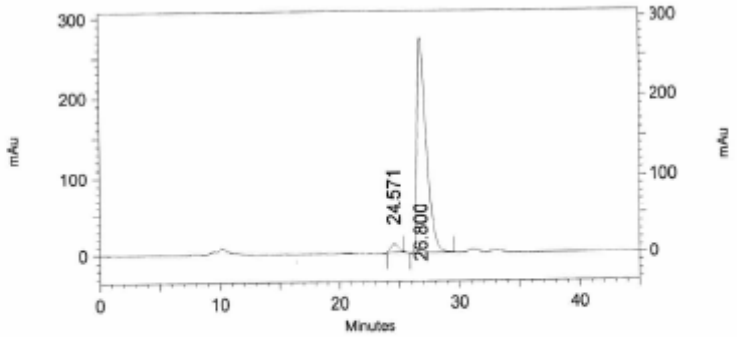
From (*S*,*S*,*S*)-**11c**, Table 3, entry 14**:**



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
24.832	2158555	4.201
27.008	49228840	95.799

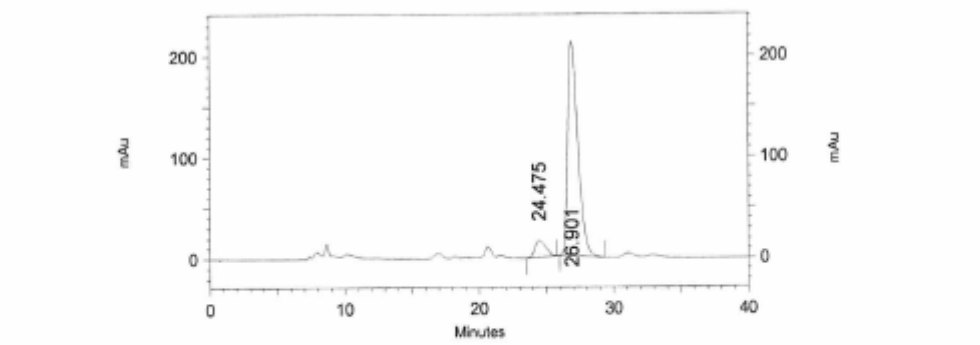
From (*S*,*S*,*S*)-**11c**, Table 3, entry 15**:**



2: 240 nm, 4 nm Results

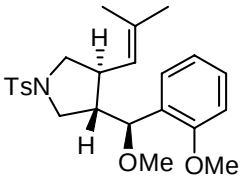
Retention Time	Area	Area Percent
24.571	494332	3.234
26.800	14790639	96.766

From (*S*,*S*,*S*)-**4c**, Table 4, entry 11**:**



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
24.475	914394	7.688
26.901	10979232	92.312

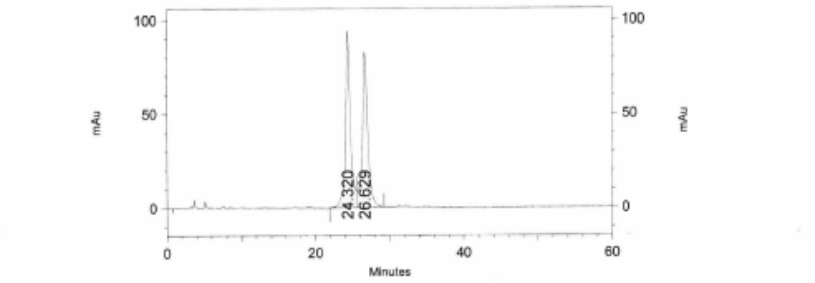


3d. Purified via silica gel flash column chromatography to give a white solid in 73% yield (hexanes:EtOAc, 90:10, Rf = 0.16). ^{1}H NMR (400MHz, $CDCl_3$): δ 7.70 (d, *J* = 8.2Hz, 1H), 7.31 (d, *J* = 8.0Hz, 1H), 7.20 (d, *J* = 7.6Hz, 1H), 6.93 (t, *J* = 7.3Hz, 1H), 6.80 (d, *J* = 8.0Hz, 1H), 4.62 (d, *J* = 9.1Hz, 1H), 4.39 (d, *J* = 5.7Hz, 1H), 3.76 (s, 3H), 3.49-3.38 (m, 2H), 3.16 (dd, *J* = 8.1, 9.8Hz, 1H), 3.11 (s, 3H), 2.83 (dt, *J* = 9.0, 16.4Hz, 1H), 2.74 (t, *J* = 9.1Hz, 1H), 2.44 (s, 3H), 2.04-2.12 (m, 1H), 1.53 (s, 3H), 1.42 (s, 3H). ^{13}C NMR (151MHz, $CDCl_3$): δ 157.1, 143.1, 134.3, 134.1, 129.5, 128.3, 127.6, 126.7, 123.9, 120.6, 110.1, 76.0, 56.8, 56.8, 55.2, 53.2, 50.3, 49.0, 39.2, 25.6, 21.5, 17.7. HRMS (EI+): calculated for $C_{24}H_{31}NO_4S$ 429.1974, found 429.1964.

HPLC trace for coumpound **3d** (Table 4, entry 1):

Method: Whelk-O1, hexanes:*i*PrOH, 85:15, 1.0 mL/min.

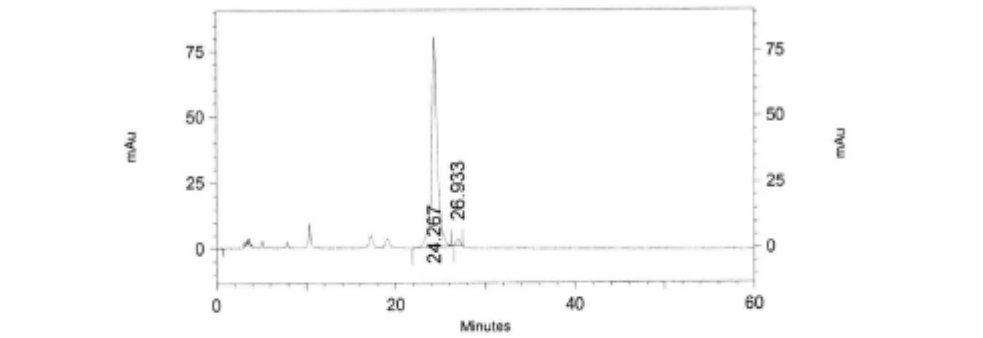
Racemic:



1: 210 nm, 4 nm Results

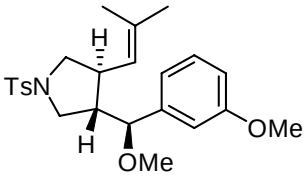
Retention Time	Area	Area Percent
24.320	4391601	51.756
26.629	4093595	48.244

From (*S*,*S*,*S*)-**11c**, Table 4, entry 1**:**



1: 211 nm, 4 nm Results

Retention Time	Area	Area Percent
24.267	3547220	98.160
26.933	66488	1.840

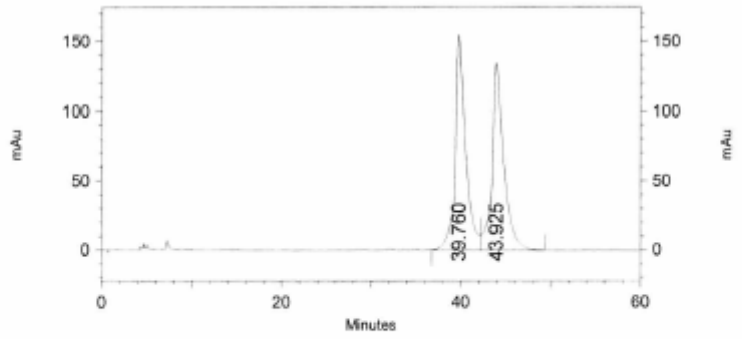


3e. Purified via silica gel flash column chromatography (hexanes:EtOAc, 90:10, Rf = 0.17). Isolated as a white solid (92%). ^{1}H NMR (400MHz, $CDCl_3$): δ 7.69 (d, *J* = 8.2Hz, 2H), 7.32 (d, *J* = 8.0Hz, 1H), 7.22 (t, *J* = 7.9Hz, 1H), 6.78 (dd, *J* = 2.6, 8.2Hz, 1H), 6.73 (d, *J* = 8.4Hz, 1H), 6.68 (bs, 1H), 4.58 (d, *J* = 9.2Hz, 1H), 3.83 (d, *J* = 1.6Hz, 1H), 3.10 (s, 3H), 3.41-3.48 (m, 2H), 3.21 (dd, *J* = 8.0, 10.0Hz, 1H), 3.13 (s, 3H), 2.84-2.75 (m, 1H), 2.72 (t, *J* = 9.1Hz, 1H), 2.44 (s, 3H), 1.90-1.98 (m, 1H), 1.58 (s, 3H), 1.42 (s, 3H). ^{13}C NMR (151MHz, $CDCl_3$): δ 159.8, 143.2, 141.9, 134.8, 133.9, 129.6, 129.4, 127.6, 123.6, 119.1, 112.9, 112.3, 82.6, 56.8, 55.2, 53.1, 52.0, 48.9, 39.5, 25.6, 21.5, 17.8. HRMS (EI+): calculated for $C_{24}H_{31}NO_4S$ 429.1974, found 429.1967.

HPLC trace for coumpound **3e**:

Method: Whelk-O1, hexanes:*i*PrOH, 85:15, 1.0 mL/min.

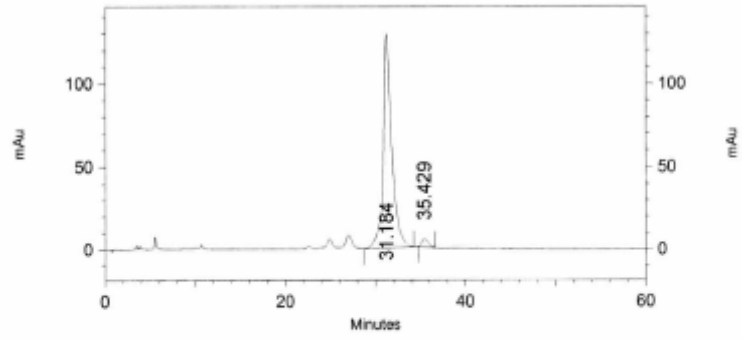
Racemic:



1: 230 nm, 4 nm Results

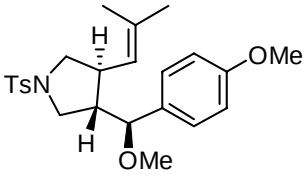
Retention Time	Area	Area Percent
39.760	12518055	50.514
43.925	12263197	49.486

From (*S*,*S*,*S*)-**11c**, Table 4, entry 2**:**



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
31.184	8526285	97.276
35.429	238789	2.724

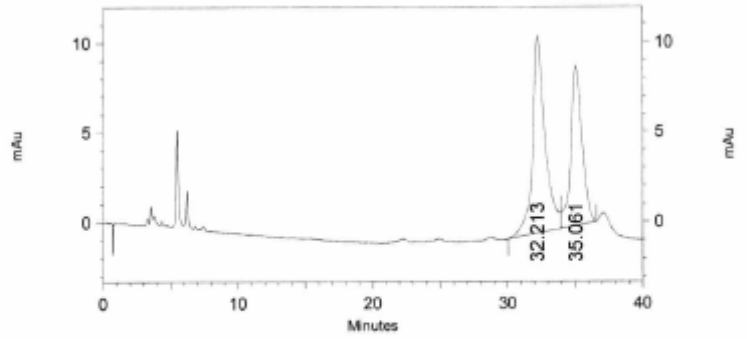


3f. Prepared by the method described above to give **3f** (90%) as a white solid. ^{1}H NMR (400MHz, $CDCl_3$): δ 7.70 (d, *J* = 8.0Hz, 2H), 7.32 (d, *J* = 8.0Hz, 2H), 7.05 (d, *J* = 8.8Hz, 2H), 6.82 (d, *J* = 8.4Hz, 2H), 4.54 (d, *J* = 9.2Hz, 1H), 3.82 (d, *J* = 7.2Hz, 1H), 3.80 (s, 3H), 3.43 (d, *J* = 8.4Hz, 2H), 3.24 (dd, *J* = 8.0, 10.0Hz 1H), 3.09 (s, 3H), 2.80-2.68 (m, 2H), 2.44 (s, 3H), 1.97-1.87 (m, 1H), 1.50 (s, 3H), 1.38 (s, 3H). ^{13}C NMR (100MHz, $CDCl_3$): δ 159.2, 143.2, 134.5, 133.7, 132.0, 129.5, 127.9, 127.6, 123.6, 113.7, 56.5, 55.3, 53.1, 52.1, 49.2, 39.5, 25.5, 21.5, 17.8. HRMS (EI+): calculated for $C_{24}H_{31}NO_4S$ 429.1974, found 429.1968.

HPLC trace for compound **3f**:

Method: Whelk-O1, hexanes:*i*PrOH, 85:15, 1.0 mL/min.

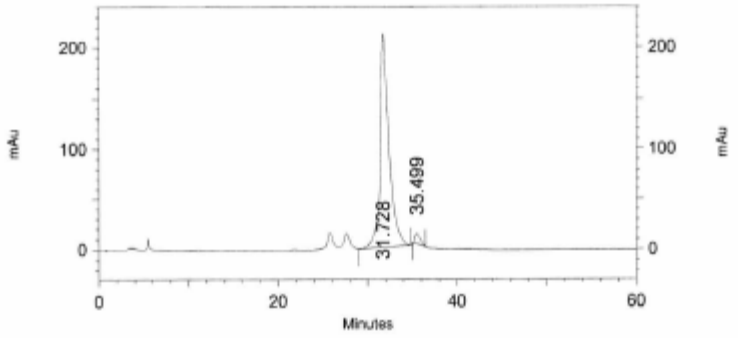
Racemic:



2: 241 nm, 4 nm Results

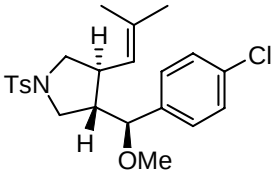
Retention Time	Area	Area Percent
32.213	705416	57.942
35.061	512031	42.058

From (*S*,*S*,*S*)-**11c**, Table 4, entry 3**:**



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
31.728	14658007	97.250
35.499	414569	2.750

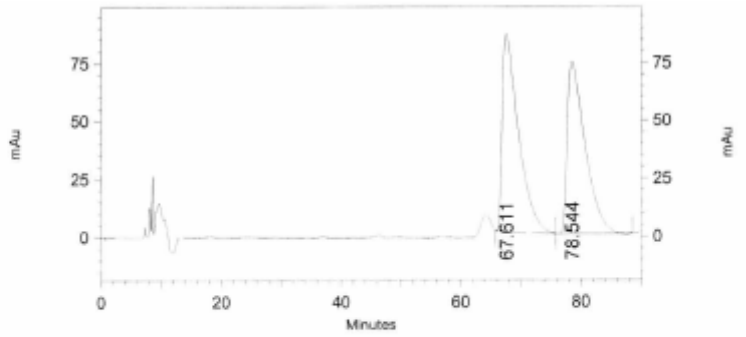


3g. Prepared by the method described above to give **3g** as a colorless oil (68%). ^{1}H NMR (400MHz, $CDCl_3$): δ 7.69 (d, *J* = 8.1Hz, 2H), 7.32 (d, *J* = 8.2Hz, 2H), 7.28 (d, *J* =8.1Hz, 2H), 7.08 (d, *J* = 8.4Hz, 2H), 4.53 (d, *J* = 9.4Hz, 1H), 3.86 (d, *J* = 5.9Hz, 1H), 3.48-3.40 (m, 1H), 3.20 (t, *J* = 8.3Hz, 1H), 3.11 (s, 3H), 2.76 (q, *J* = 9.2Hz, 1H), 2.69 (t, *J* = 9.1Hz, 1H), 2.45 (s, 3H), 1.90 (dt, *J* = 8.3, 14.5Hz, 1H), 1.51 (s, 3H), 1.41 (s, 3H). ^{13}C NMR (151MHz, $CDCl_3$): δ 143.3, 138.7, 135.0, 134.0, 133.6, 129.6, 128.6, 128.1, 127.6, 82.6, 56.8, 53.1, 51.9, 49.0, 39.6, 26.1, 21.8, 18.3. HRMS (EI+): calculated for $C_{23}H_{28}ClNO_3S$ 433.1478, found 433.1477.

HPLC trace for compound **3g**:

Method: Chiracel OD, hexanes:*i*PrOH, 99:01, 0.5 mL/min.

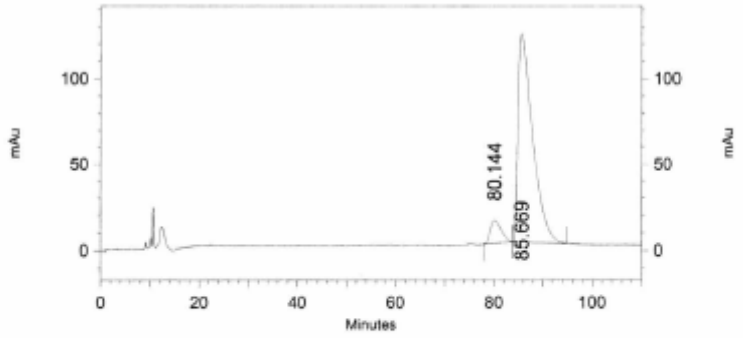
Racemic:



1: 230 nm, 4 nm Results

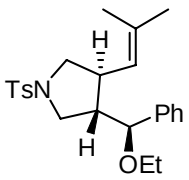
Retention Time	Area	Area Percent
67.611	15999840	51.375
78.544	15143286	48.625

From (*S*,*S*,*S*)-**11c**, Table 4, entry 4**:**



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
80.144	1986603	7.395
85.669	24877707	92.605



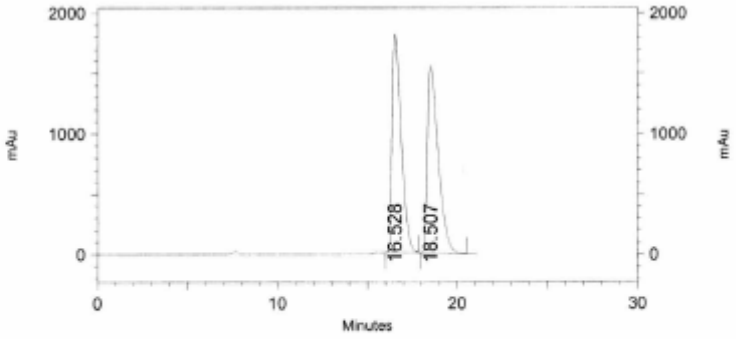
3h. Prepared by the method described above to give the product (90%) as a colorless oil. Isolated via silica gel flash column chromatography (pet. Ether:DCM, 50:50, Rf = 0.2). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.69 (d, *J* = 8.1Hz, 2H), 7.31-7.21 (m, 5H), 4.12 (d, *J* = 8.0Hz, 2H), 4.55 (d, *J* = 9.0Hz, 1H), 3.96 (d, *J* = = 5.7Hz, 1H), 3.48 (q, *J* = 8.7Hz, 2H), 3.35-3.25 (m, 1H), 3.21-3.07 (m, 2H), 2.84-2.72 (m, 2H), 2.16 (s, 3H), 1.93 (dt, *J* = 8.4, 14.1Hz, 1H), 1.57 (s, 3H), 1.50 (s, 3H), 1.09 (t, *J* = 6.9Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 43.2, 140.9, 134.9, 133.9, 129.5, 128.3, 128.1, 127.6, 126.6, 123.5, 80.6,

64.3, 53.2, 52.1, 48.9, 39.4, 25.6, 21.5, 17.8, 15.2. HRMS (EI+): calculated for $C_{24}H_{31}NO_3S$ 413.2025, found 431.2019.

HPLC trace for compound **3h** (Table 4, entry 5):

Method: Chiracel OD, hexanes:*i*PrOH, 93:07, 0.5 mL/min.

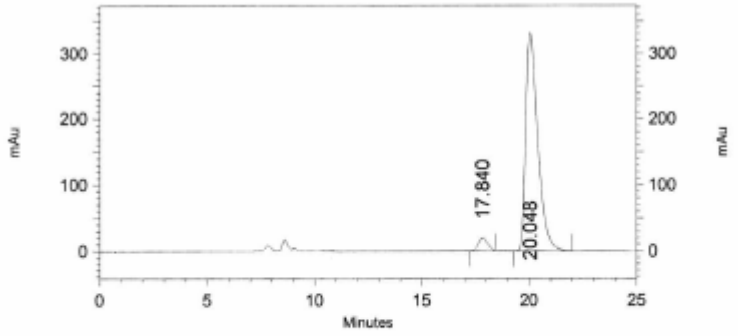
Racemic:



1: 230 nm, 4 nm Results

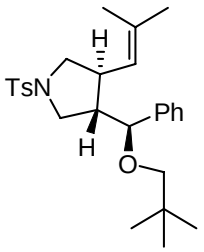
Retention Time	Area	Area Percent
16.528	62940095	49.396
18.507	64478512	50.604

From (*S*,*S*,*S*)-**11c**, Table 4, entry 5**:**



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
17.840	549787	4.049
20.048	13027009	95.951



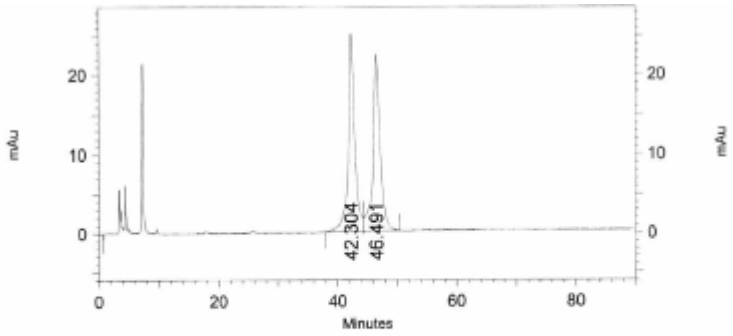
3i. Isolated via silica gel flash column chromatography (pet. Ether:DCM, 50:50, Rf = 0.45) as a colorless oil (71%). ^{1}H NMR (300MHz, $CDCl_3$): δ 7.68 (d, *J* = 8.4Hz, 2H), 7.31-7.22 (m, 5H), 7.11 (d. *J* = 9.6Hz, 2H), 4.47 (d, *J* = 8.2Hz, 1H), 3.95 (d, *J* = 4.3Hz, 1H), 3.48 (q, *J* = 5.2Hz, 1H), 3.44 (d, *J* =

9.4Hz, 1H), 3.20 (t, *J* = 8.0Hz, 1H), 2.90 (d, *J* = 8.3Hz, 1H), 2.82-2.74 (m, 2H), 2.78 (d, *J* =8.3Hz, 1H), 2.42 (s, 3H), 1.94-1.90 (m, 1H), 1.58 (s, 3H), 1.44 (s, 3H), 0.82 (s, 9H). ^{13}C NMR (126MHz, $CDCl_3$): δ 143.2, 141.9, 135.2, 133.9, 129.6, 128.5, 128.3, 127.5, 126.3, 123.4, 79.6, 79.1, 53.3, 52.7, 39.3, 32.1, 26.8, 25.7, 21.5, 18.0. HRMS (EI+): calculated for $C_{27}H_{37}NO_3S$ 455.2500, found 455.2455.

HPLC trace for compound **3i**:

Method: Whelk-O1, hexanes:*i*PrOH, 95:05, 1.0 mL/min.

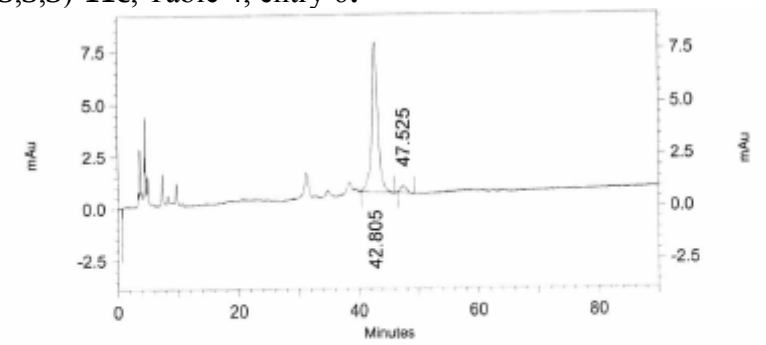
Racemic:



1: 230 nm, 4 nm Results

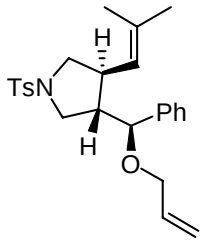
Retention Time	Area	Area Percent
42.304	1946926	50.706
46.491	1892678	49.294

From (*S*,*S*,*S*)-**11c**, Table 4, entry 6**:**



1: 235 nm, 4 nm Results

Retention Time	Area	Area Percent
42.805	504214	96.500
47.525	18286	3.500

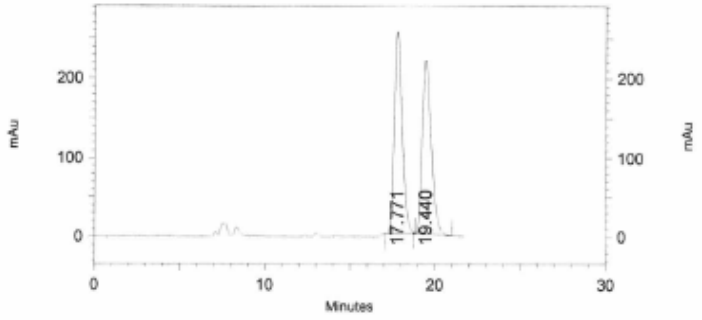


3j. Prepared by the method described above to give **3j** as a colorless oil (84%). Isolated via silica gel flash column chromatography (petroleum Ether:DCM, 50:50, Rf = 0.2). ^{1}H NMR (600MHz, $CDCl_3$): δ 7.69 (d, *J* = 7.8Hz, 2H), 7.32-7.23 (m, 5H), 7.25 (d, *J* = 7.2Hz, 2H), 5.83-5.77 (m, 1H), 5.14 (d, *J* = 17.4Hz, 1H), 5.11 (d, *J* = 10.8Hz, 1H), 4.56 (d, *J* = 9.6Hz, 1H), 4.05 (d, *J* = 9.6Hz, 1H), 3.83 (dd, *J* = 5.4, 12.6Hz, 1H), 3.60 (dd, *J* = 5.4, 12.6Hz, 1H), 3.51-3.45 (m, 2H), 3.24 (dd, *J* = 7.8, 10.2Hz, 1H), 2.81-2.71 (m, 2H), 2.44 (s, 3H), 2.01-1.96 (m, 1H), 1.49 (s, 3H), 1.37 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 143.2, 140.3, 134.8, 134.5, 134.0, 129.6, 128.4, 127.8, 127.6, 126.7, 123.5, 116.6, 80.4, 69.6, 53.2, 52.1, 49.1, 39.5, 25.5, 21.5, 17.8. HRMS (EI+): calculated for $C_{25}H_{31}NO_3S$ 425.2025, found 425.1984.

HPLC traces for compound **3j**:

Method: Chiracel OD, hexanes:*i*PrOH (93:07), 0.5 mL/min

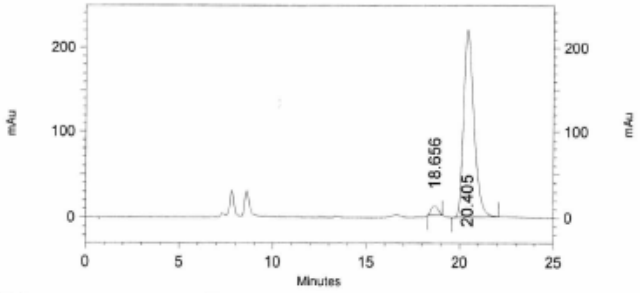
Racemic:



1: 230 nm, 4 nm Results

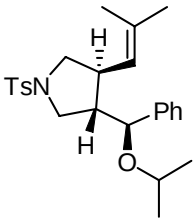
Retention Time	Area	Area Percent
17.771	8192393	50.630
19.440	7988392	49.370

From (*S*,*S*,*S*)-**11c**, Table 4, entry 7**:**



2: 210 nm, 4 nm Results

Retention Time	Area	Area Percent
18.656	276401	3.169
20.405	8445498	96.831

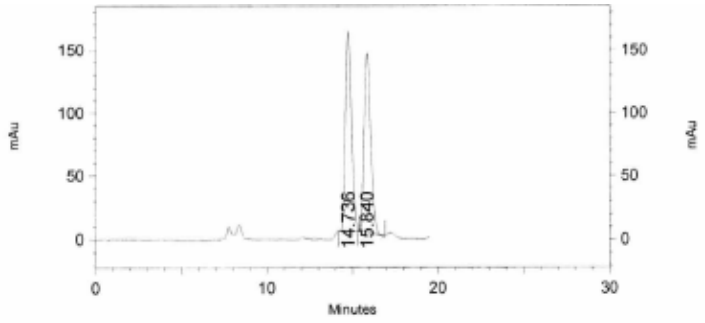


3k. Prepared by the method described above to give **3k** as a colorless oil (81%). Isolated via silica gel flash column chromatography (petroleum ether:DCM, 50:50, Rf = 0.23). ^{1}H NMR (600MHz, $CDCl_3$): δ 7.69 (d, *J* = 7.8Hz, 2H), 7.31 (d, *J* = 7.8Hz, 2H), 7.28-7.26 (m, 2H), 7.22 (d, *J* = 7.2Hz, 1H), 7.16 (d, *J* = 7.2Hz, 2H), 4.54 (d, *J* = 9.0Hz, 1H), 4.14 (d, *J* = 5.4Hz, 1H), 3.50-3.46 (m, 2H), 3.39-3.25 (m, 1H), 3.20 (t, *J* = 8.4Hz, 1H), 2.76-2.70 (m, 1H), 2.66 (t, *J* = 9.6Hz, 1H), 2.43 (s, 3H), 1.98-1.92 (m, 1H), 1.49 (s, 3H), 1.37 (s, 3H), 1.03 (d, *J* = 6.0Hz, 3H), 0.94 (d, *J* = 6.0Hz, 3H). ^{13}C NMR (151MHz, $CDCl_3$): δ 20.7, 21.0, 21.2, 30.9, 42.7, 46.7, 50.4, 52.1, 124.2, 125.2, 125.7, 128.4, 129.3, 129.4, 135.9, 142.4. HRMS (EI+): calculated for $C_{25}H_{33}NO_3S$ 427.2181, found 427.2139.

HPLC traces for compound **3k**:

Method: Chiracel OD, hexanes:*i*PrOH (93:07), 0.5 mL/min

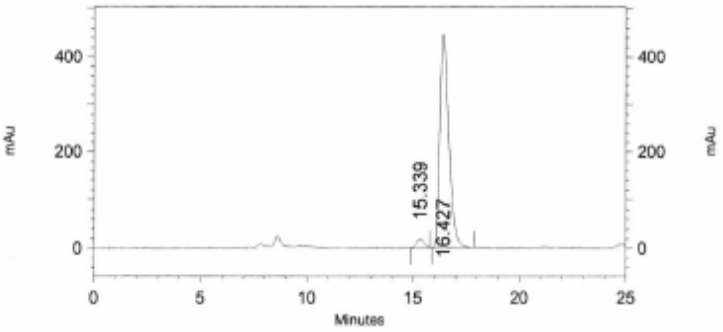
Racemic:



1: 230 nm, 4 nm Results

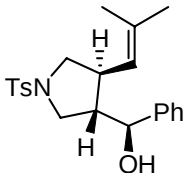
Retention Time	Area	Area Percent
14.736	3873496	50.545
15.840	3790028	49.455

From (*S*,*S*,*S*)-**11c**, Table 4, entry 8**:**



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
15.339	419781	3.112
16.427	13070357	96.888

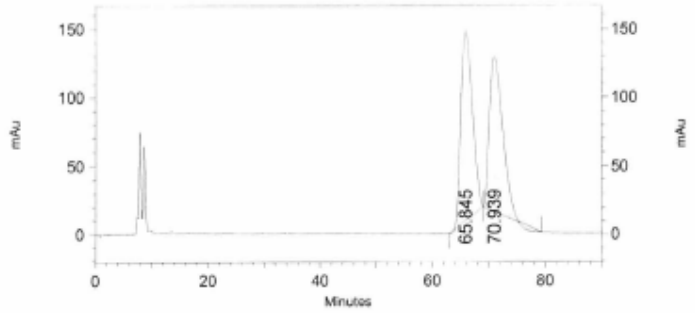


3l. Prepared by the method described above to give **3l** as a white solid (85%). Isolated via silica gel flash column chromatography (hexanes:EtOAc 80:20, Rf = 0.04). ^{1}H NMR (300MHz, $CDCl_3$): δ 7.68 (d, *J* = 8.2Hz, 2H), 7.32-7.19 (m, 7H), 4.62 (d, *J* = 8.6Hz, 1H), 4.48 (d, *J* = 5.6Hz, 1H), 3.49-3.41 (m, 2H), 3.21 (t, *J* = 8.1Hz, 1H), 2.86-2.70 (m, 2H), 2.43 (s, 3H), 2.03 (dt, *J* = 8.2, 14.1Hz, 1H), 1.74 (bs, 2H), 1.51 (s, 3H), 1.40 (s, 3H). ^{13}C NMR (126MHz, $CDCl_3$): δ 143.3, 142.8, 135.2, 133.6, 129.6, 128.4, 127.8, 127.6, 125.9, 123.4, 73.3, 53.2, 52.1, 48.5, 39.5, 25.6, 21.5, 17.9. HRMS (EI+): calculated for $C_{22}H_{27}NO_3S$ 385.1712, found 385.1705.

HPLC traces for compound **3l**:

Method: Chiracel OD, hexanes:*i*PrOH (93:07), 0.5 mL/min

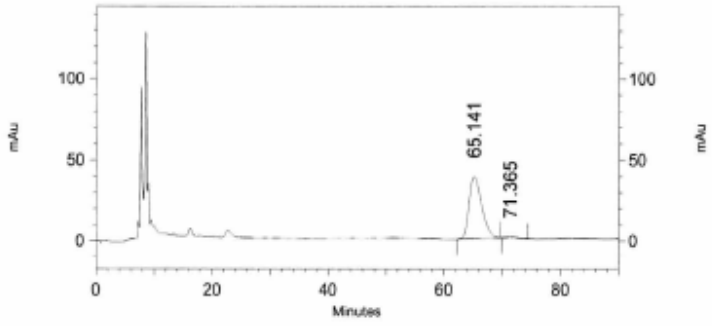
Racemic:



2: 210 nm, 4 nm Results

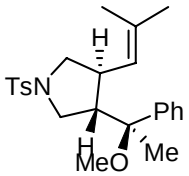
Retention Time	Area	Area Percent
65.845	19546499	51.756
70.939	18220401	48.244

From (*S*,*S*,*S*)-**11c**, Table 4, entry 9**:**



1: 220 nm, 4 nm Results

Retention Time	Area	Area Percent
65.141	5785155	97.988
71.365	118787	2.012

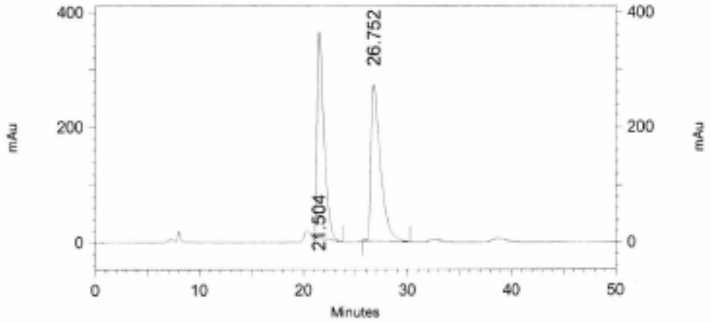


3m. Prepared by the method described above to give **3m** as a colorless oil (83%). Isolated via silica gel flash column chromatography (hexanes:EtOAc, 90:10, Rf = 0.27). ^{1}H NMR (400MHz, $CDCl_3$): δ 7.65 (d, *J* = 8.2Hz, 2H), 7.32-7.26 (m, 4H), 7.22-7.19 (m, 3H), 4.49 (d, *J* = 9.3Hz, 1H), 3.41-3.35 (m, 2H), 3.01 (s, 3H), 3.04-2.99 (m, 1H), 2.83-2.76 (m, 1H), 2.56 (t, *J* = 8.9Hz, 1H), 2.45 (s, 3H), 2.12 (dt, *J* = 8.4, 16.6Hz, 1H), 1.49 (s, 3H), 1.42 (s, 3H), 1.39 (s, 3H). ^{13}C NMR (151MHz, $CDCl_3$): δ 143.3, 143.2, 133.3, 132.3, 129.5, 128.0, 127.8, 127.1, 126.4, 125.6, 79.5, 56.6, 53.8, 50.3, 49.3, 38.7, 25.4, 21.5, 18.8, 17.8. HRMS (EI+): calculated for $C_{24}H_{31}NO_3S$ 413.2025, found 413.2022.

HPLC traces for compound **3m**:

Method: Chiracel OD, hexanes:*i*PrOH (93:07), 0.5 mL/min

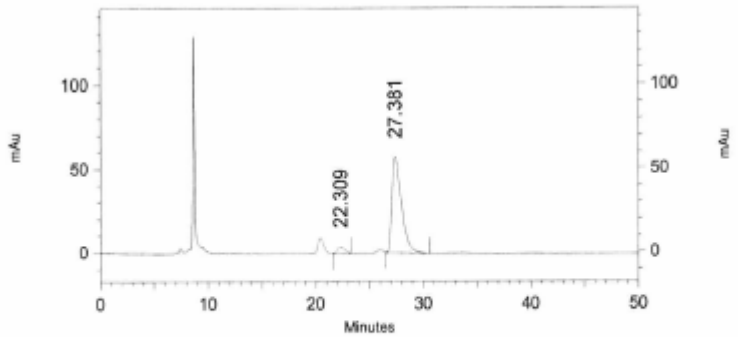
Racemic:



1: 230 nm, 4 nm Results

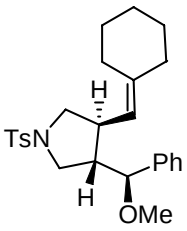
Retention Time	Area	Area Percent
21.504	16692720	49.033
26.752	17351166	50.967

From (*S*,*S*,*S*)-**11c**, Table 4, entry 12**:**



2: 242 nm, 4 nm Results

Retention Time	Area	Area Percent
22.309	166272	4.561
27.381	3479023	95.439

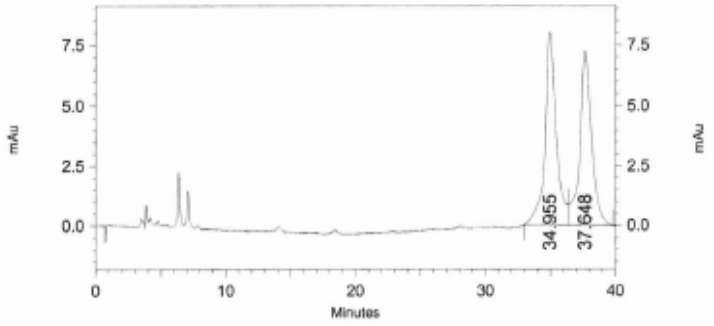


3n. Prepared by the method described above to give **3n** as a colorless oil (76%). Isolated via silica gel flash column chromatography (hexanes:EtOAc, 90:10, Rf = 0.25). ^{1}H NMR (400MHz, $CDCl_3$): δ 7.68 (d, *J* = 8.2Hz, 2H), 7.32-7.24 (m, 5H), 7.13 (d, *J* = 8.4Hz, 2H), 4.52 (d, *J* = 9.2Hz, 1H), 3.86 (d, *J* = 5.7Hz, 1H), 3.48-3.40 (m, 2H), 3.20 (dd, *J* = 8.1, 10.0Hz, 1H), 3.10 (s, 3H), 2.78 (dt, *J* = 9.0, 16.4Hz, 1H), 2.71 (t, *J* = 9.2Hz, 1H), 2.42 (s, 3H), 1.98-1.86 (m, 5H), 1.46-1.38 (m, 6H). All spectroscopic data was in agreement with previoulsy reported data.[10] HRMS (ESI): calculated for $C_{26}H_{33}NO_3SNa$ [M + Na] 462.2073, found 462.2065.

HPLC traces for compound **3n**:

Method: Whelk-O1, hexanes:*i*PrOH, 90:10, 1.0 mL/min.

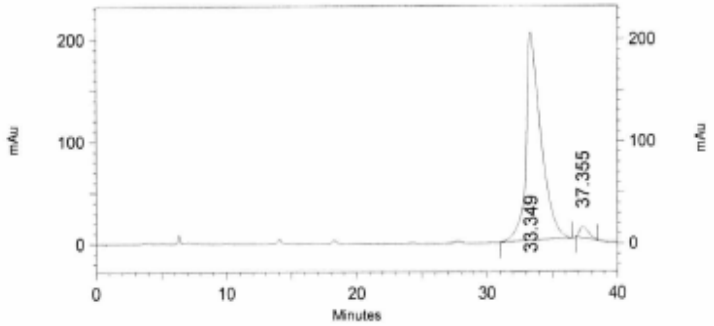
Racemic:



1: 244 nm, 4 nm Results

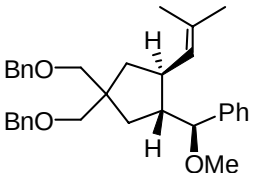
Retention Time	Area	Area Percent
34.955	482894	51.248
37.648	459371	48.752

From (*S*,*S*,*S*)-**11c**, Table 4, entry 13**:**



1: 240 nm, 4 nm Results

Retention Time	Area	Area Percent
33.349	16214107	96.919
37.355	515449	3.081

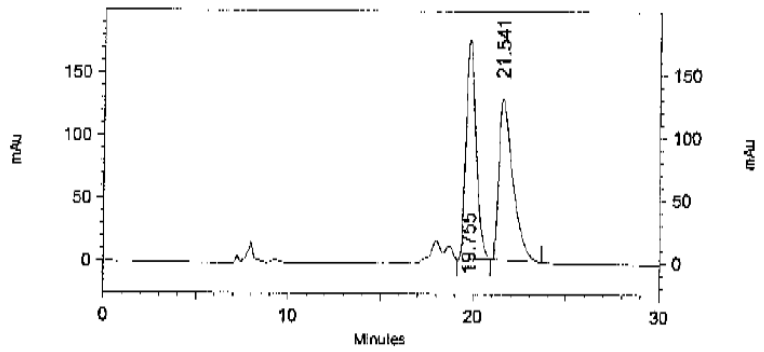


3o. Prepared by the method described above to give **3o** as a clear oil (80%). Isolated via silica gel flash column chromatography (hexanes:EtOAc, 90:10). ^{1}H NMR (400MHz, $CDCl_3$): δ 7.29-7.16 (m, 15H), 5.19-4.97 (m, 4H), 4.76 (d, *J* = 9.6Hz, 1H), 3.96 (d, *J* = 4.2Hz, 1H), 3.16 (s, 3H), 2.91-2.78 (m, 1H), 2.53-2.21 (m, 1H), 1.92-1.76 (m, 2h), 1.58 (s, 3H), 1.53 (s, 3H). ^{13}C NMR (125MHz, $CDCl_3$): δ 172.3, 141.4, 135.7, 135.5, 133.1, 124.4 (2C), 128.1, 128.0, 128.0, 127.8, 127.1, 126.8, 126.6, 82.8, 66.9, 58.3, 56.9, 53.1, 40.9, 40.5, 34.3, 30.9, 25.7, 18.0.

HPLC traces for compound **3o**:

Method: Chiracel IA, hexanes:*i*PrOH (95:05), 1.0 mL/min

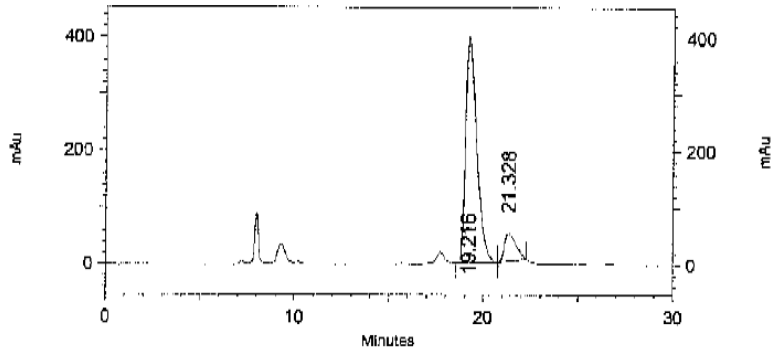
Racemic:



2: 219 nm, 4 nm Results

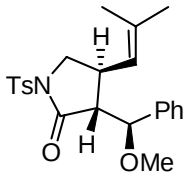
Retention Time	Area	Area Percent
19.755	6568991	49.802
21.541	6621180	50.198

From (*S*,*S*,*S*)-**11c**, Table 4, entry 14**:**



1: 220 nm, 4 nm Results

Retention Time	Area	Area Percent
19.216	16147601	88.639
21.328	2069744	11.361

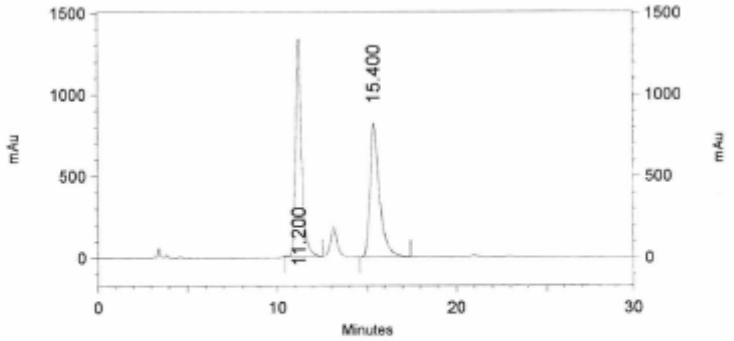


13a. Prepared by the method described above to give **13a** as a white solid (93%). Isolated via silica gel flash column chromatography (hexanes:EtOAc, 80:20, Rf = 0.14). ^{1}H NMR (400MHz, $CDCl_3$): δ 7.85 (d, *J* = 8.3Hz, 2H), 7.33 (d, *J* = 8.2Hz, 2H), 7.23-7.13 (m, 5H), 4.98 (d, *J* = 9.1Hz, 1H), 4.56 (d, *J* = 3.8Hz, 1H), 3.50 (dd, *J* = 7.6, 9.5Hz, 1H), 3.24 (s, 3H), 3.18 (dt, *J* = 7.2, 9.6Hz, 1H), 2.94 (dt, *J* = 3.8, 8.1Hz, 1H), 2.46 (s, 3H), 1.67 (s, 3H), 1.55 (s, 3H). ^{13}C NMR (125MHz, $CDCl_3$): δ 172.1, 145.0, 137.7, 135.2, 135.0, 129.6, 128.3, 128.1, 127.9, 126.9, 123.9, 81.6, 57.2, 56.1, 50.6, 33.1, 25.6, 21.7, 18.0. HRMS (EI+): calculated for $C_{23}H_{27}NO_4S$ 413.1661, found 413.1660.

HPLC traces for compound **13a**:

Method: Chiracel IA, hexanes:*i*PrOH (95:05), 1.0 mL/min

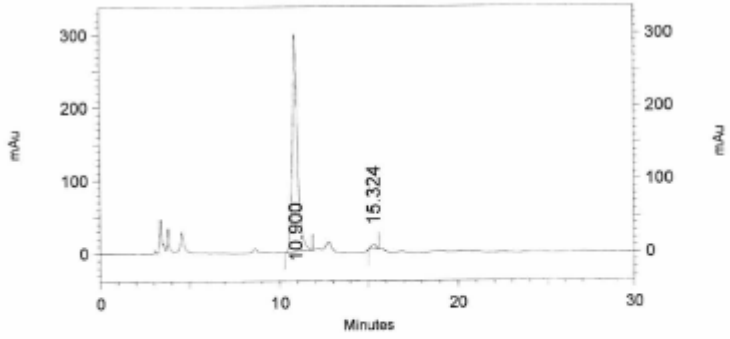
Racemic:



1: 210 nm, 4 nm Results

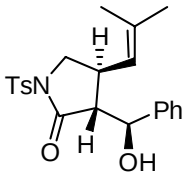
Retention Time	Area	Area Percent	Lambda Max
11.200	29720571	49.596	207
15.400	30084632	50.304	207

From (*S*,*S*,*S*)-**11c:**

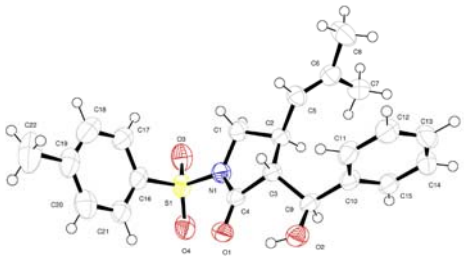


1: 210 nm, 4 nm Results

Retention Time	Area	Area Percent	Lambda Max
10.900	6286580	98.231	206
15.324	113182	1.769	206



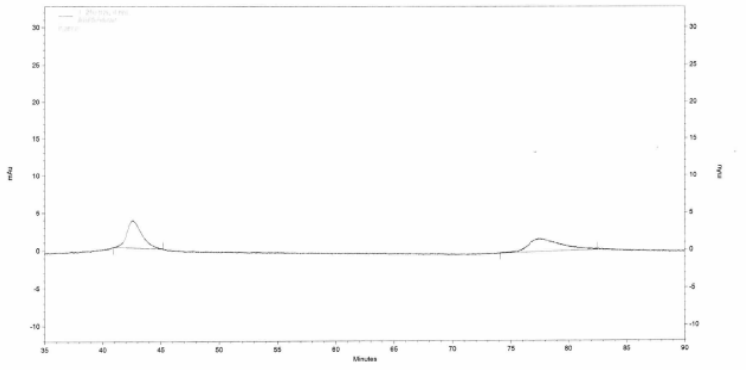
13b. Prepared by the method described above to give **13b** as a crystalline solid (81%). Isolated via silica gel flash column chromatography (hexanes:EtOAc, 80:20, Rf = 0.04). ^{1}H NMR (400MHz, $CDCl_3$): δ 7.93 (d, *J* = 8.3Hz, 2H), 7.38 (d, *J* = 8.1Hz, 2H), 7.27-7.21 (m, 5H), 4.75 (d, *J* = 8.2Hz, 1H), 4.43 (d, *J* = 9.2Hz, 1H), 3.89 (d, *J* = 8.3Hz, 1H), 3.19 (t, *J* = 9.6Hz, 1H), 2.87 (dt, *J* = 9.1Hz, 1H), 2.58 (dd, *J* = 8.2, 10.5Hz, 1H), 2.48 (s, 3H), 1.35 (s, 6H). ^{13}C NMR (125MHz, $CDCl_3$): δ 175.0, 145.5, 139.5, 135.7, 134.7, 129.8, 128.2, 128.1, 126.7, 122.5, 74.7, 55.5, 34.6, 25.2, 21.7, 17.8. HRMS (EI+): calculated for $C_{22}H_{25}NO_4S$ 399.1504, found 399.1463. See bellow for a solid state structure of **13b**:



HPLC traces for compound **13b**:

Method: Whelk-O1, hexanes:*i*PrOH, 80:20, 1.0 mL/min.

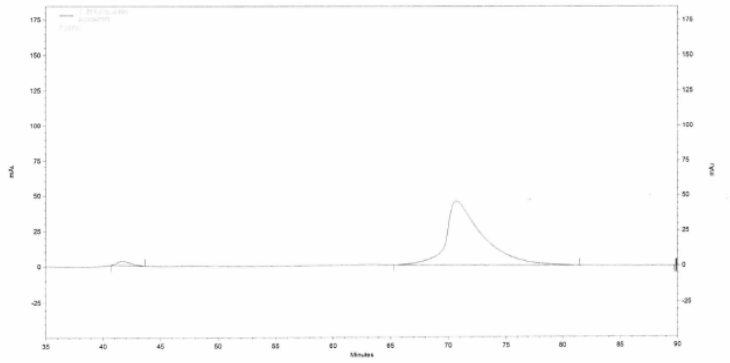
Racemic:



1: 210 nm, 4 nm Results

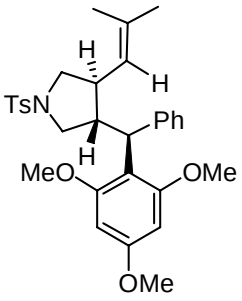
Retention Time	Area	Area Percent
42.645	328034	50.627
77.461	319912	49.373

From (*S*,*S*,*S*)-**11c:**



1: 211 nm, 4 nm Results

Retention Time	Area	Area Percent
41.669	237287	2.380
70.709	9734304	97.620

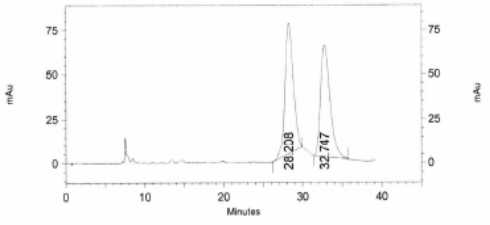


3p. Prepared by the method described above to give **3p** as a white solid (73%). Isolated via silica gel flash column chromatography. ^{1}H NMR (400MHz, $CDCl_3$): δ 7.65 (d, *J* = 8.2Hz, 2H), 7.32-7.27 (m, 4H), 7.08-7.02 (m, 2H), 7.01-6.97 (m, 1H), 6.04 (s, 2H), 4.47 (d, *J* = 9.7Hz, 1H), 4.27 (d, *J* = 11.1Hz, 1H), 3.73 (s, 3H), 3.69 (bs, 6H), 3.41 (dd, *J* = 7.4Hz, 1H), 3.27 (dd, *J* = 7.7, 9.7Hz, 1H), 3.20-3.12 (m, 1H), 2.88-2.77 (m, 2H), 2.63-2.54 (m, 1H), 2.45 (s, 3H), 1.25 (s, 3H), 1.16 (s, 3H). ^{13}C NMR (151MHz, $CDCl_3$): δ 159.7, 143.5, 143.0, 133.9, 132.2, 129.4, 128.8, 127.7, 127.6, 127.4, 125.6, 125.5, 112.5, 91.3, 55.2, 53.6, 52.6, 46.2, 44.6, 43.6, 29.8, 25.4, 21.5, 17.6. HRMS (EI+): calculated for $C_{31}H_{37}NO_4S$ 535.2392, found 535.2378.

HPLC traces for compound **3p**:

Method: Chiracel OD, hexanes:*i*PrOH (93:07), 0.5 mL/min

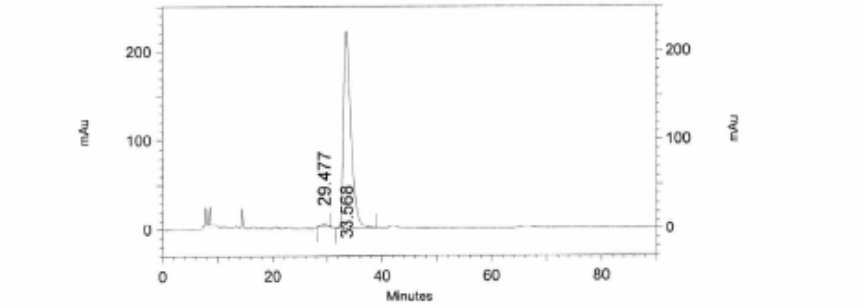
Racemic:



1: 230 nm, 4 nm Results

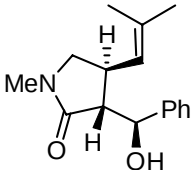
Retention Time	Area	Area Percent
28.208	5411855	50.873
32.747	5226065	49.127

From (*S*,*S*,*S*)-**11c:**



2: 210 nm, 4 nm Results

Retention Time	Area	Area Percent
29.477	346689	1.605
33.568	21256665	98.395

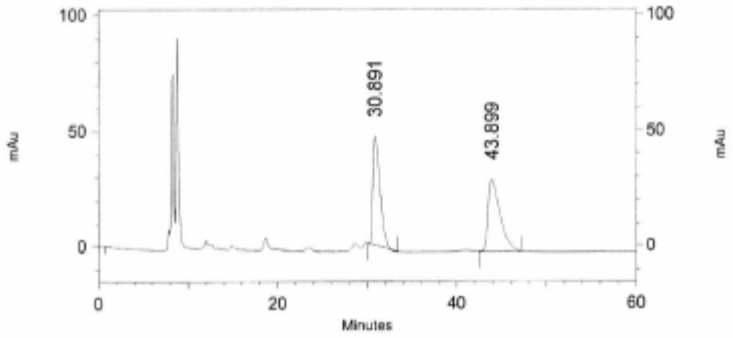


15. Prepared by the method described above to give **15** as a crystalline solid (93%). Isolated via silica gel flash column chromatography (hexanes:EtOAc, 60:40, Rf = 0.3). ^{1}H NMR (400MHz, $CDCl_3$): δ 7.35-7.25 (m, 5H), 4.71 (d, *J* = 9.5Hz, 1H), 4.55 (d, *J* = 9.3Hz, 1H), 4.15 (bs, 1H), 3.33 (t, *J* = 9.6Hz, 1H), 2.94 (t, *J* = 8.7Hz, 1H), 2.90 (s, 3H), 2.82 (dt, *J* = 9.1, 17.8Hz, 1H), 2.57-2.53 (t, *J* = 9.4Hz, 1H), 1.33 (s, 3H), 1.22 (s, 3H). ^{13}C NMR (125MHz, $CDCl_3$): δ 140.4, 133.9, 128.1, 128.0, 127.4, 124.1, 76.3, 53.8, 53.5, 34.7, 29.4, 25.2, 17.6. HRMS (ESI): calculated for $C_{16}H_{21}NO_2Na$ [M + Na] 282.1470, found 282.1461.

HPLC traces for compound **15**:

Method: Chiracel OD, hexanes:*i*PrOH (85:15), 0.5 mL/min

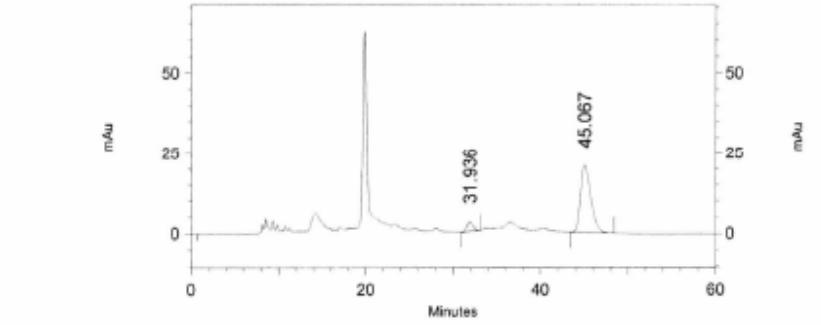
Racemic:



2: 224 nm, 4 nm Results

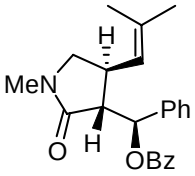
Retention Time	Area	Area Percent
30.891	2663899	47.848
43.899	2903490	52.152

From (*S*,*S*,*S*)-**11c:**

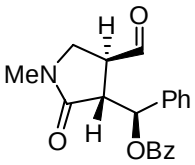


1: 220 nm, 4 nm Results

Retention Time	Area	Area Percent
31.936	126858	7.027
45.067	1678403	92.973



16. To a solution of **15** (0.07mmols, 17mg), DMAP (10 mol %, 1mg) and pyridine (1.3mmols, 0.1mL) in dichloromethane (2mL) was added benzoyl chloride (0.09mmols, 0.02mL). The reaction mixture was stirred at room temeperture for 12h. After this period the crude reaction mixture was partitioned with water and dichloromethane (3 × 30mL). The combined organic layer was dried over $MgSO_4$, filtered and the filtrate was concentrated under vacuum. The product (**16**) was then isolated via silica gel flash column chromatography (hexanes:EtOAc, 60:40, Rf = 0.4) in 85% (20mg). ^{1}H NMR (400MHz, $CDCl_3$): δ 8.14 (d, *J* = 8.0Hz, 2H), 7.62 (t, *J* = 7.4Hz, 1H), 7.48 (t, *J* = 7.9Hz, 2H), 7.33-7.22 (m, 5H), 4.70 (d, *J* = 9.6Hz, 1H), 4.54 (d, *J* = 9.2Hz, 1H), 3.29 (t, *J* = 8.4Hz, 1H), 2.92 (t, *J* = 8.4Hz, 1H), 2.85 (s, 3H), 2.83-2.78 (m, 1H), 2.54 (t, *J* = 9.2Hz, 1H), 1.31 (s, 3H), 1.20 (s, 3H). ^{13}C NMR (125MHz, $CDCl_3$): δ 176.3, 171.4, 150.3, 140.3, 133.9, 133.6, 130.2, 128.4, 128.1, 128.0, 127.4, 124.1, 53.8, 53.5, 34.7, 29.5, 25.2, 17.6.



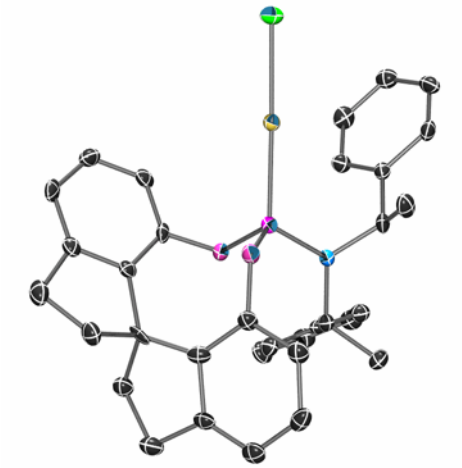
17. Ozone was bubbled into a solution of **16** (0.06mmols, 20mg) in dichloromethane (5mL) at −78°C. After the reaction was complete nitrogen was bubled for 5 mins and then Me_2S was added at −78°C. The reaction was allowed to reach room temperature and stirred for and additional 3h. The crude reaction mixture was concentrated and purified via silica gel flash column chromatography (petroleum ether: ethyl acetate, 1:1) to give a colorless solid in 94% (18mg). ^{1}H NMR (400MHz, $CDCl_3$): δ 9.72 (s, 1H), 8.09 (dd, *J* = 1.5, 7.2Hz, 2H), 7.64-7.58 (m, 1H), 7.51-7.32 (m, 7H), 6.65 (d, *J* = 4.2Hz, 1H), 3.56-

3.49 (m, 2H), 3.29-3.22 (m, 1H), 2.80-2.73 (m, 1H), 2.73 (s, 3H). All other spectroscopic data was in complete agreement with those reported in the literature.[17]

[17] Xu, W.; Kong, A.; Lu, X. *J. Org. Chem.* **2006**, *71*, 3854. Rh: Cao, P.; Wang, B.; Zhang, Y. *J. Am. Chem. Soc.* **2000**, *122*, 6490.

3. Crystallographic Data

3.1 Crystallographic data for (*R*,*R*,*R*)-**9a**

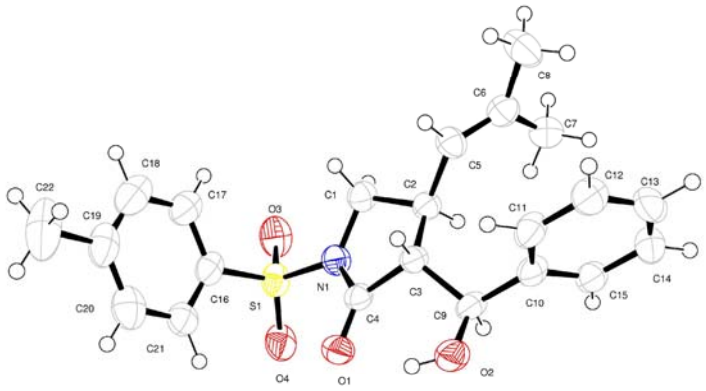


A colorless block 0.20 x 0.20 x 0.15 mm in size was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 133(2) K using phi and omega scans. Crystal-to-detector distance was 60 mm and exposure time was 10 seconds per frame using a scan width of 0.3°. Data collection was 99.9% complete to 25.00° in θ. A total of 25523 reflections were collected covering the indices, -13<=*h*<=10, -14<=*k*<=14, -24<=*l*<=25. 5353 reflections were found to be symmetry independent, with an R_{int} of 0.0319. Indexing and unit cell refinement indicated a primitive, orthorhombic lattice. The space group was found to be P2(1)2(1)2(1) (No. 19). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by direct methods (SIR-97) produced a complete heavy-atom phasing model consistent with the proposed structure. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-97). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-97. Absolute stereochemistry was unambiguously confirmed to be *S* at P1 and *R* at C18 and C26, respectively.

Table 1. Crystal data and structure refinement for toste25.

X-ray ID	toste25	
Sample/notebook ID	R-SIPHOS-PE-AuCl	
Empirical formula	C33 H32 Au Cl N O2 P	
Formula weight	737.98	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 11.4404(14) Å	α= 90°.
	b = 12.1589(15) Å	β= 90°.
	c = 20.835(3) Å	γ = 90°.
Volume	2898.1(6) $Å^3$	
Z	4	
Density (calculated)	1.691 Mg/m^3	
Absorption coefficient	5.255 mm^{-1}	
F(000)	1456	
Crystal size	0.20 x 0.20 x 0.15 mm^3	
Crystal color/habit	colorless block	
Theta range for data collection	2.44 to 25.44°.	
Index ranges	-13<=h<=10, -14<=k<=14, -24<=l<=25	
Reflections collected	25523	
Independent reflections	5353 [R(int) = 0.0319]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.5062 and 0.4196	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5353 / 0 / 354	
Goodness-of-fit on F^2	1.004	
Final R indices [I>2sigma(I)]	R1 = 0.0218, wR2 = 0.0441	
R indices (all data)	R1 = 0.0296, wR2 = 0.0460	
Absolute structure parameter	-0.002(5)	
Largest diff. peak and hole	1.725 and -0.731 $e.Å^{-3}$	

3.2 Crystallographic data for **13b**

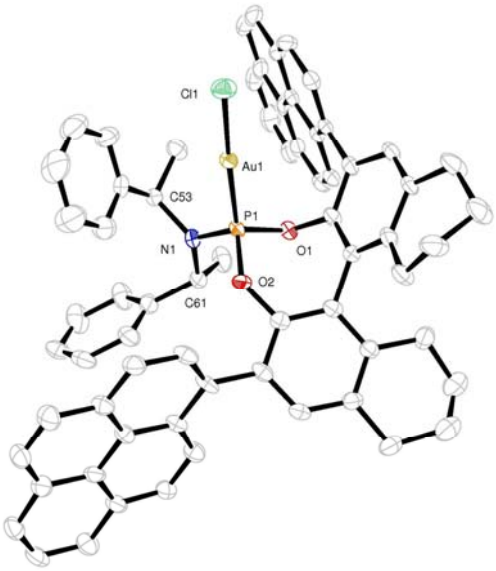


A colorless prism 0.08 x 0.06 x 0. 04 mm in size was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K using phi and omega scans. Crystal-to-detector distance was 60 mm and exposure time was 10 seconds per frame using a scan width of 1.0°. Data collection was 99.5% complete to 67.00° in θ. A total of 11648 reflections were collected covering the indices, -12<=*h*<=12, -10<=*k*<=9, -14<=*l*<=13. 3612 reflections were found to be symmetry independent, with an R_{int} of 0.0610. Indexing and unit cell refinement indicated a primitive, monoclinic lattice. The space group was found to be P2(1) (No. 4). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by direct methods (SIR-2008) produced a complete heavy-atom phasing model consistent with the proposed structure. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-97). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-97. Absolute stereochemistry was unambiguously determined to be *S* at C2, *R* at C3, and *S* at C9.

Table 1. Crystal data and structure refinement for toste30.

X-ray ID	toste30	
Sample/notebook ID	AG04-186H	
Empirical formula	C22 H25 N O4 S	
Formula weight	399.49	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 10.4997(8) Å	α= 90°.
	b = 8.3483(6) Å	β= 91.036(5)°.
	c = 11.8012(7) Å	γ = 90°.
Volume	1034.26(12) $Å^3$	
Z	2	
Density (calculated)	1.283 Mg/m^3	
Absorption coefficient	1.615 mm^{-1}	
F(000)	424	
Crystal size	0.08 x 0.06 x 0.04 mm^3	
Crystal color/habit	colorless prism	
Theta range for data collection	3.75 to 67.85°.	
Index ranges	-12<=h<=12, -10<=k<=9, -14<=l<=13	
Reflections collected	11648	
Independent reflections	3612 [R(int) = 0.0610]	
Completeness to theta = 67.00°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9382 and 0.8816	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3612 / 1 / 257	
Goodness-of-fit on F^2	1.031	
Final R indices [I>2sigma(I)]	R1 = 0.0624, wR2 = 0.1567	
R indices (all data)	R1 = 0.0763, wR2 = 0.1679	
Absolute structure parameter	-0.06(3)	
Largest diff. peak and hole	0.494 and -0.192 $e.Å^{-3}$	

3.3 Crystallographic data for (*R*,*R*,*R*)-**11a**

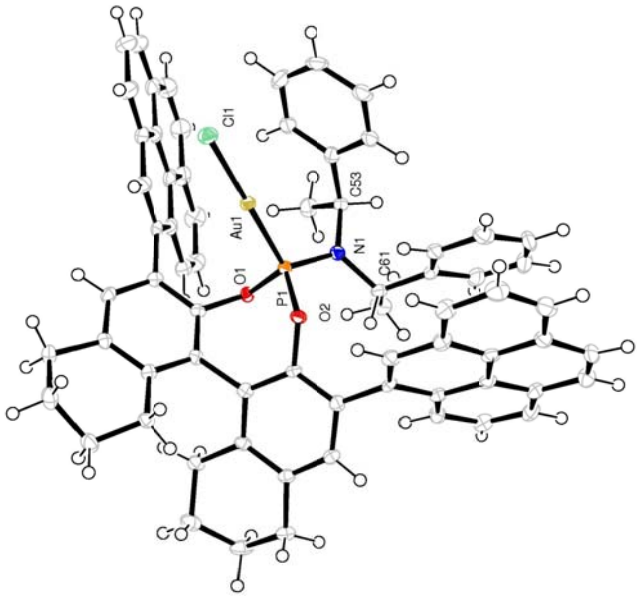


A colorless needle 0.12 x 0.08 x 0.04 mm in size was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K using phi and omega scans. Crystal-to-detector distance was 60 mm and exposure time was 5 seconds per frame using a scan width of 1.0°. Data collection was 99.5% complete to 67.00° in θ. A total of 53424 reflections were collected covering the indices, -15<=*h*<=15, -13<=*k*<=15, -21<=*l*<=21. 9977 reflections were found to be symmetry independent, with an R_{int} of 0.0297. Indexing and unit cell refinement indicated a primitive, monoclinic lattice. The space group was found to be P2(1) (No. 4). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by direct methods (SIR-97) produced a complete heavy-atom phasing model consistent with the proposed structure. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-97). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-97. Absolute stereochemistry was unambiguously determined to be *S* at P1 and *R* at C53 and C61, respectively.

Table 1. Crystal data and structure refinement for toste29.

X-ray ID	toste29	
Sample/notebook ID	H_8-pyrenyl-phosphoramid-AuCl	
Empirical formula	C69 H56 Au Cl3 N O2 P	
Formula weight	1265.43	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 13.2972(7) Å	α= 90°.
	b = 13.2921(7) Å	β= 102.863(3)°.
	c = 17.5488(9) Å	γ = 90°.
Volume	3023.9(3) $Å^3$	
Z	2	
Density (calculated)	1.390 Mg/m^3	
Absorption coefficient	6.384 mm^{-1}	
F(000)	1276	
Crystal size	0.12 x 0.08 x 0.04 mm^3	
Crystal color/habit	colorless needle	
Theta range for data collection	2.58 to 68.28°.	
Index ranges	-15<=h<=15, -13<=k<=15, -21<=l<=21	
Reflections collected	53424	
Independent reflections	9977 [R(int) = 0.0297]	
Completeness to theta = 67.00°	99.5 %	
Absorption correction	Analytical	
Max. and min. transmission	0.7843 and 0.5146	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9977 / 1 / 696	
Goodness-of-fit on F^2	1.151	
Final R indices [I>2sigma(I)]	R1 = 0.0418, wR2 = 0.1263	
R indices (all data)	R1 = 0.0437, wR2 = 0.1280	
Absolute structure parameter	-0.043(9)	
Largest diff. peak and hole	2.236 and -1.220 e.$Å^{-3}$	

3.4 Crystallographic data for (*S*,*S*,*S*)-**11b**

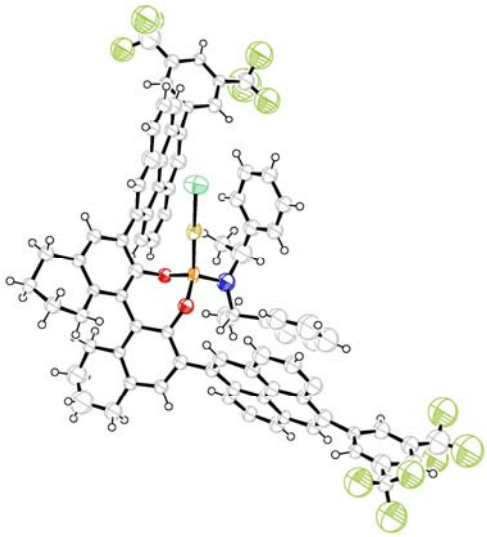


A colorless prism 0.29 x 0.12 x 0.11 mm in size was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K using phi and omega scans. Crystal-to-detector distance was 60 mm and exposure time was 5 seconds per frame using a scan width of 1.0°. Data collection was 99.9% complete to 67.00° in θ. A total of 40990 reflections were collected covering the indices, -10<=*h*<=10, -21<=*k*<=21, -19<=*l*<=19. 9052 reflections were found to be symmetry independent, with an R_{int} of 0.0411. Indexing and unit cell refinement indicated a primitive, monoclinic lattice. The space group was found to be P2(1) (No. 4). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by Patterson methods (DIRDIF-2008) produced a complete heavy-atom phasing model consistent with the proposed structure. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-97). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-97. Absolute stereochemistry was unambiguously determined to be *R* at P(1) and *S* at C(53) and C(61), respectively.

Table 1. Crystal data and structure refinement for toste31.

X-ray ID	toste31	
Sample/notebook ID	AG04-169	
Empirical formula	C68 H54 Au Cl N O2 P	
Formula weight	1180.51	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 8.5886(3) Å	α= 90°.
	b = 18.2238(6) Å	β= 95.129(2)°.
	c = 16.1210(5) Å	γ = 90°.
Volume	2513.11(14) $Å^3$	
Z	2	
Density (calculated)	1.560 Mg/m^3	
Absorption coefficient	6.681 mm^{-1}	
F(000)	1192	
Crystal size	0.29 x 0.12 x 0.11 mm^3	
Crystal color/habit	colorless prism	
Theta range for data collection	2.75 to 68.22°.	
Index ranges	-10<=h<=10, -21<=k<=21, -19<=l<=19	
Reflections collected	40990	
Independent reflections	9052 [R(int) = 0.0411]	
Completeness to theta = 67.00°	99.9 %	
Absorption correction	Analytical	
Max. and min. transmission	0.5269 and 0.2475	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9052 / 1 / 669	
Goodness-of-fit on F^2	1.019	
Final R indices [I>2sigma(I)]	R1 = 0.0216, wR2 = 0.0520	
R indices (all data)	R1 = 0.0226, wR2 = 0.0525	
Absolute structure parameter	-0.037(4)	
Largest diff. peak and hole	0.762 and -0.531 $e.Å^{-3}$	

3.5 Crystallographic data for (*S*,*S*,*S*)-**11c**

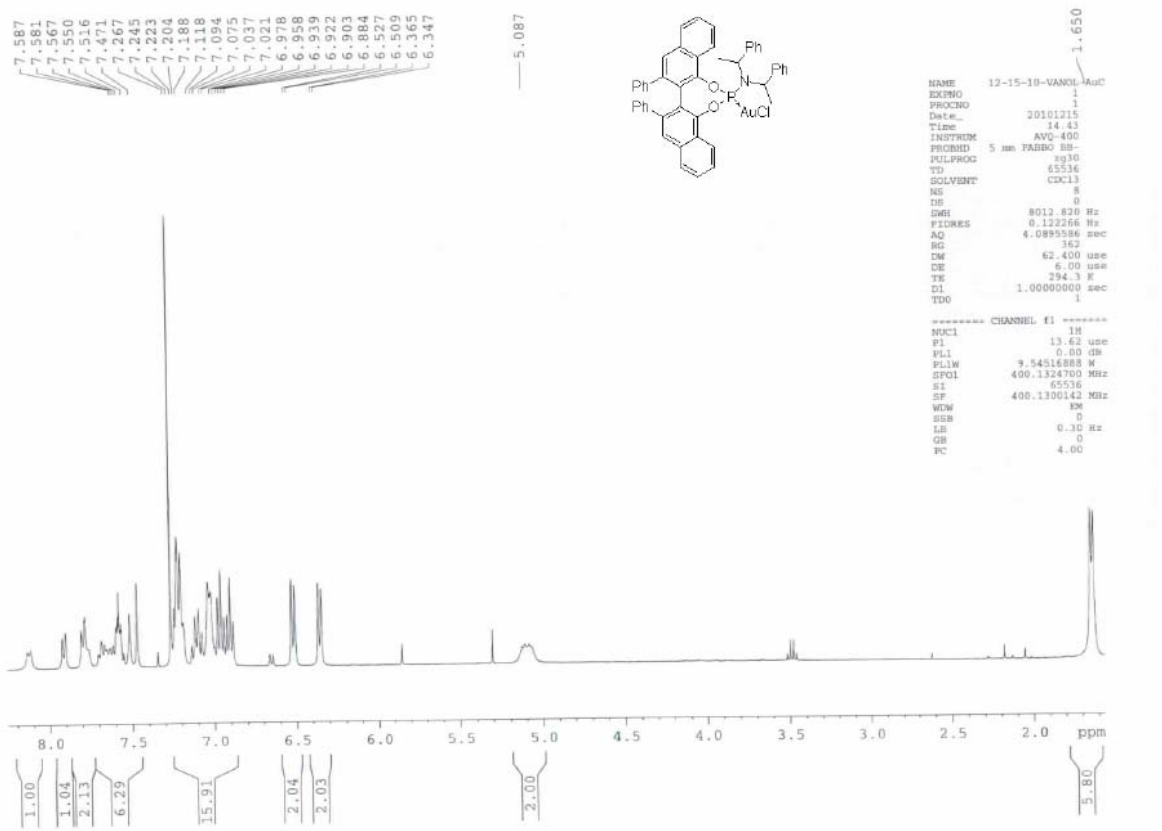


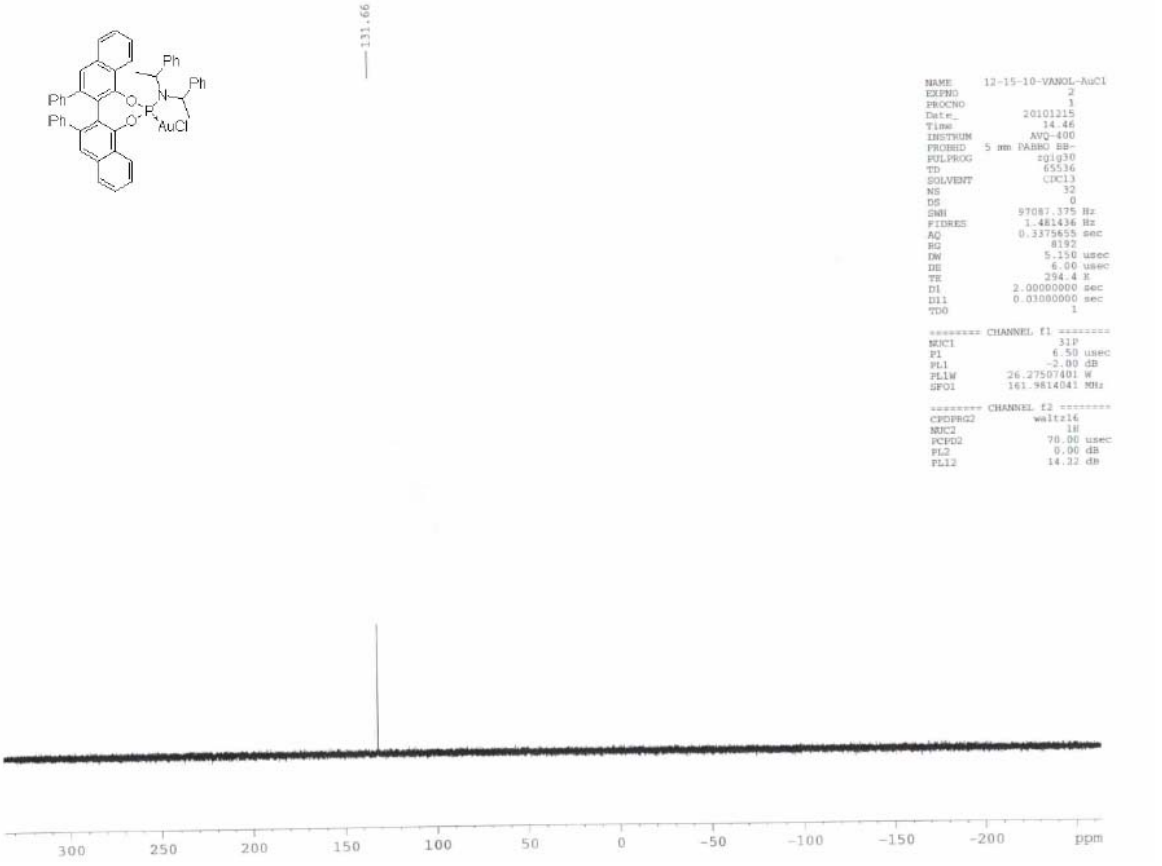
A colorless blade 0.15 x 0.06 x 0.04 mm in size was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K using phi and omega scans. Crystal-to-detector distance was 60 mm and exposure time was 10 seconds per frame using a scan width of 1.0°. Data collection was 100.0% complete to 50.00° in θ. A total of 85358 reflections were collected covering the indices, -8<=*h*<=8, -18<=*k*<=20, -36<=*l*<=44. 8009 reflections were found to be symmetry independent, with an R_{int} of 0.0789. Indexing and unit cell refinement indicated a primitive, orthorhombic lattice. The space group was found to be P2(1)2(1)2(1) (No. 19). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by charge-flipping methods (SUPERFLIP) produced a complete heavy-atom phasing model consistent with the proposed structure. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-97). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-97. Absolute stereochemistry was unambiguously determined to be *R* at P(1) and *S* at C(69) and C(77), respectively.

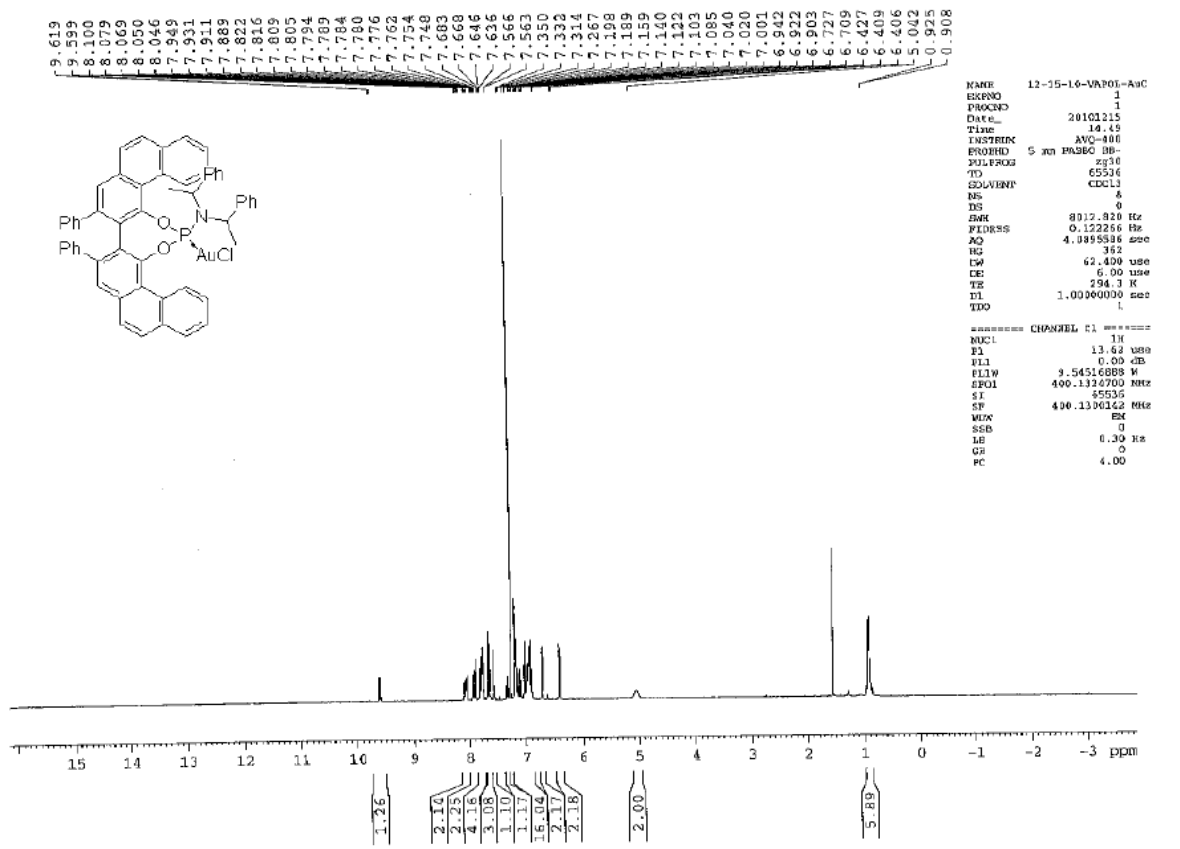
Table 1. Crystal data and structure refinement for toste32.

X-ray ID	toste32	
Sample/notebook ID	AG05-28	
Empirical formula	C84 H57 Au Cl F12 N O2 P	
Formula weight	1603.69	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 8.3457(5) Å	α= 90°.
	b = 20.6561(12) Å	β= 90°.
	c = 44.304(2) Å	γ = 90°.
Volume	7637.6(8) $Å^3$	
Z	4	
Density (calculated)	1.395 Mg/m^3	
Absorption coefficient	4.785 mm^{-1}	
F(000)	3212	
Crystal size	0.15 x 0.06 x 0.04 mm^3	
Crystal color/habit	colorless blade	
Theta range for data collection	1.99 to 50.52°.	
Index ranges	-8<=h<=8, -18<=k<=20, -36<=l<=44	
Reflections collected	85358	
Independent reflections	8009 [R(int) = 0.0789]	
Completeness to theta = 50.00°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8316 and 0.5338	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8009 / 26 / 405	
Goodness-of-fit on F^2	1.078	
Final R indices [I>2sigma(I)]	R1 = 0.1130, wR2 = 0.2939	
R indices (all data)	R1 = 0.1330, wR2 = 0.3096	
Absolute structure parameter	0.06(3)	
Largest diff. peak and hole	2.951 and -1.459 $e.Å^{-3}$	

4. Selected Spectal Data



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DE 6.00 usec
TE 294.1 K
D1 1.00000000 sec
TD0 1
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SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
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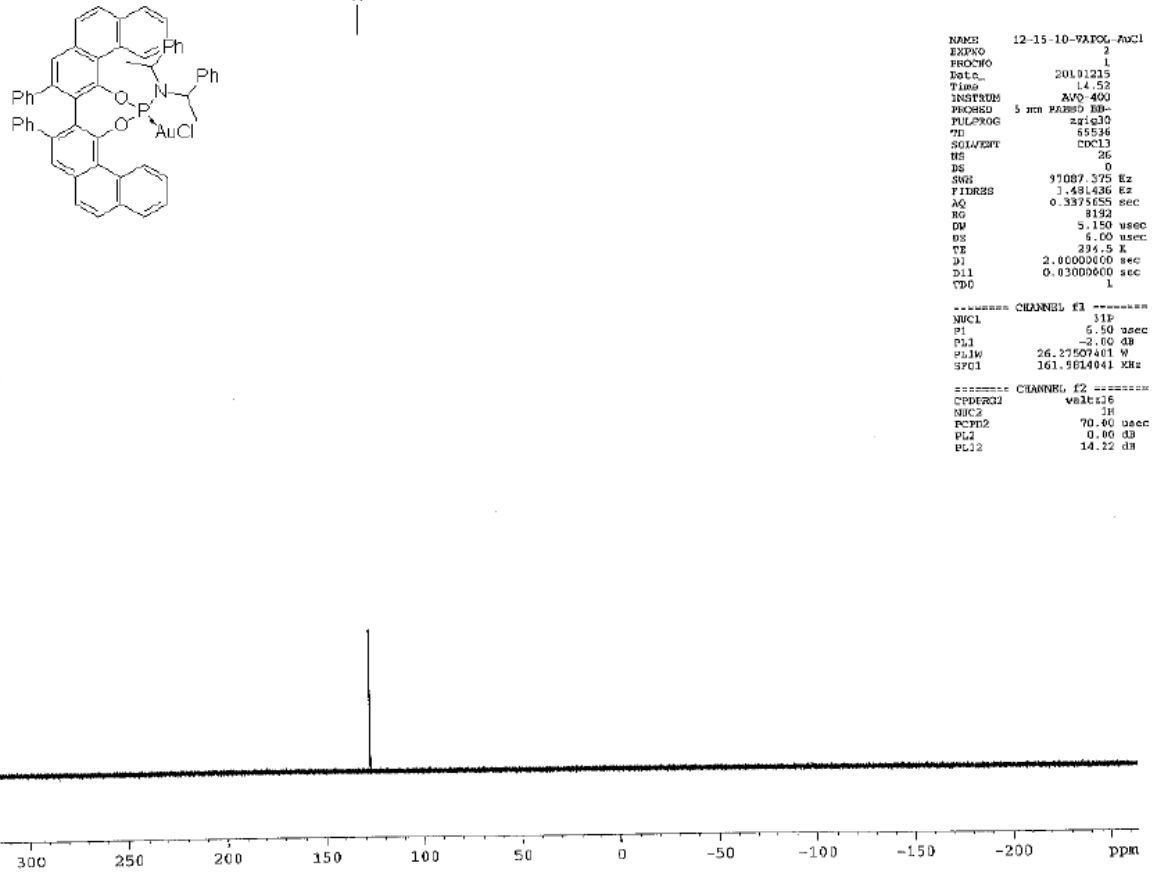
2.00
5.89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PROCNO 1
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PULPROG zgig30
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SOLVENT CDCl3
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FIDRES 1.481436 Hz
AQ 0.3375655 sec
RG 8192
DW 5.150 usec
DE 6.00 usec
TE 294.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
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NUC1 31P
P1 6.50 usec
PL1 -2.00 dB
PL1W 26.27507401 W
SFO1 161.9614041 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
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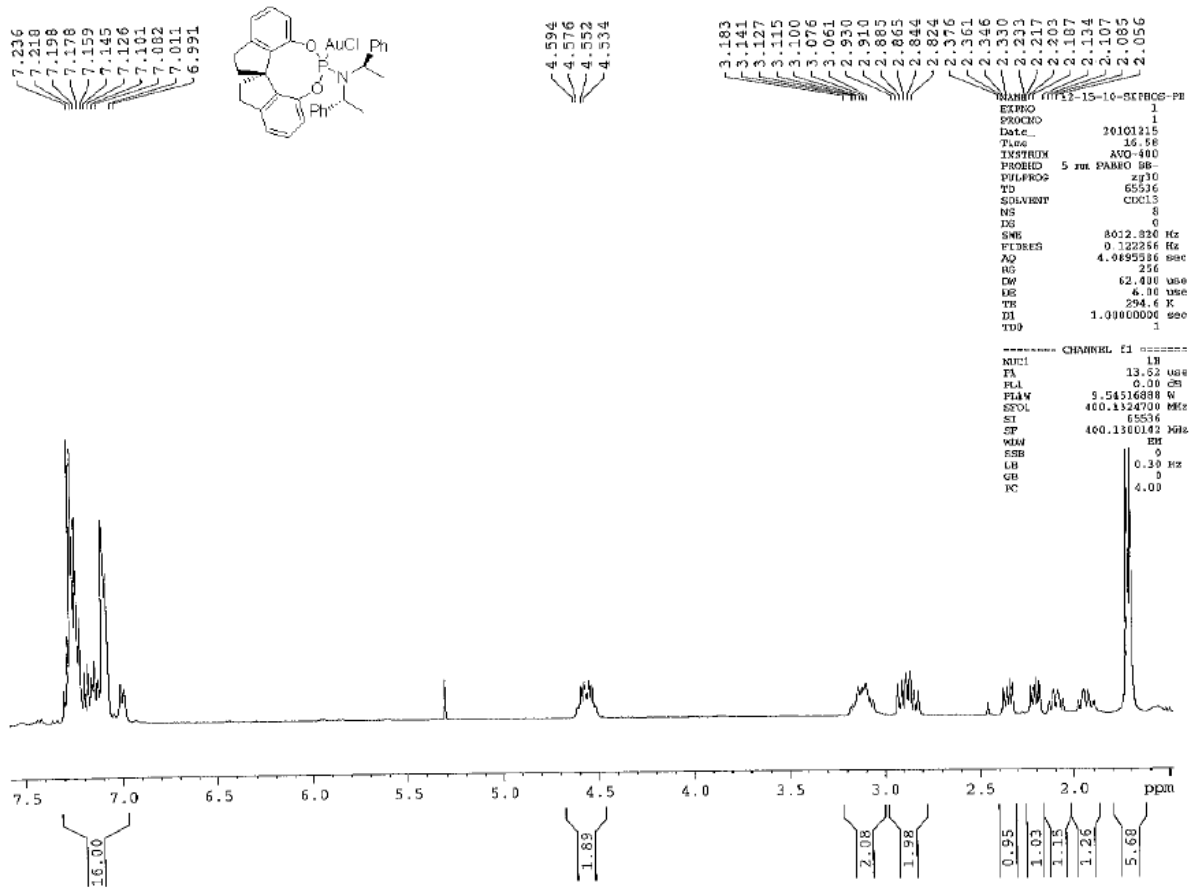
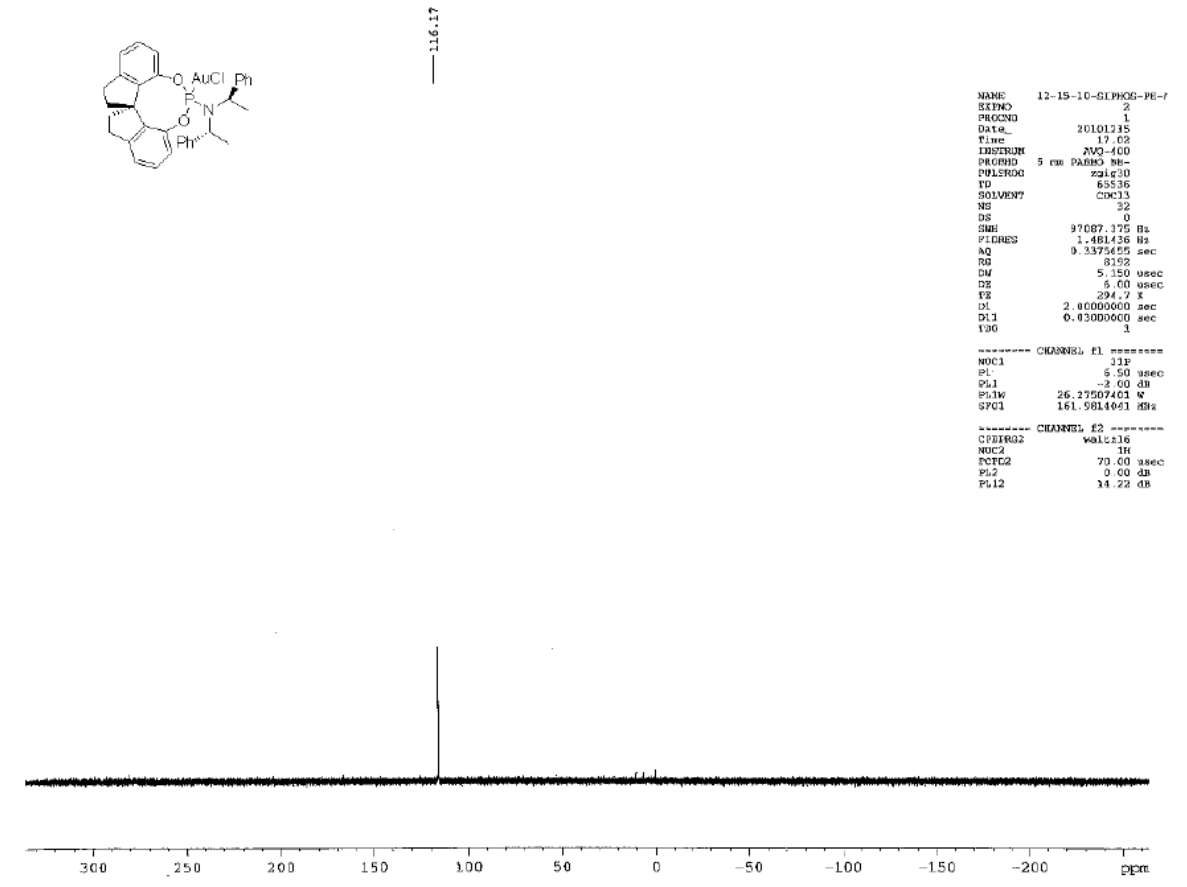
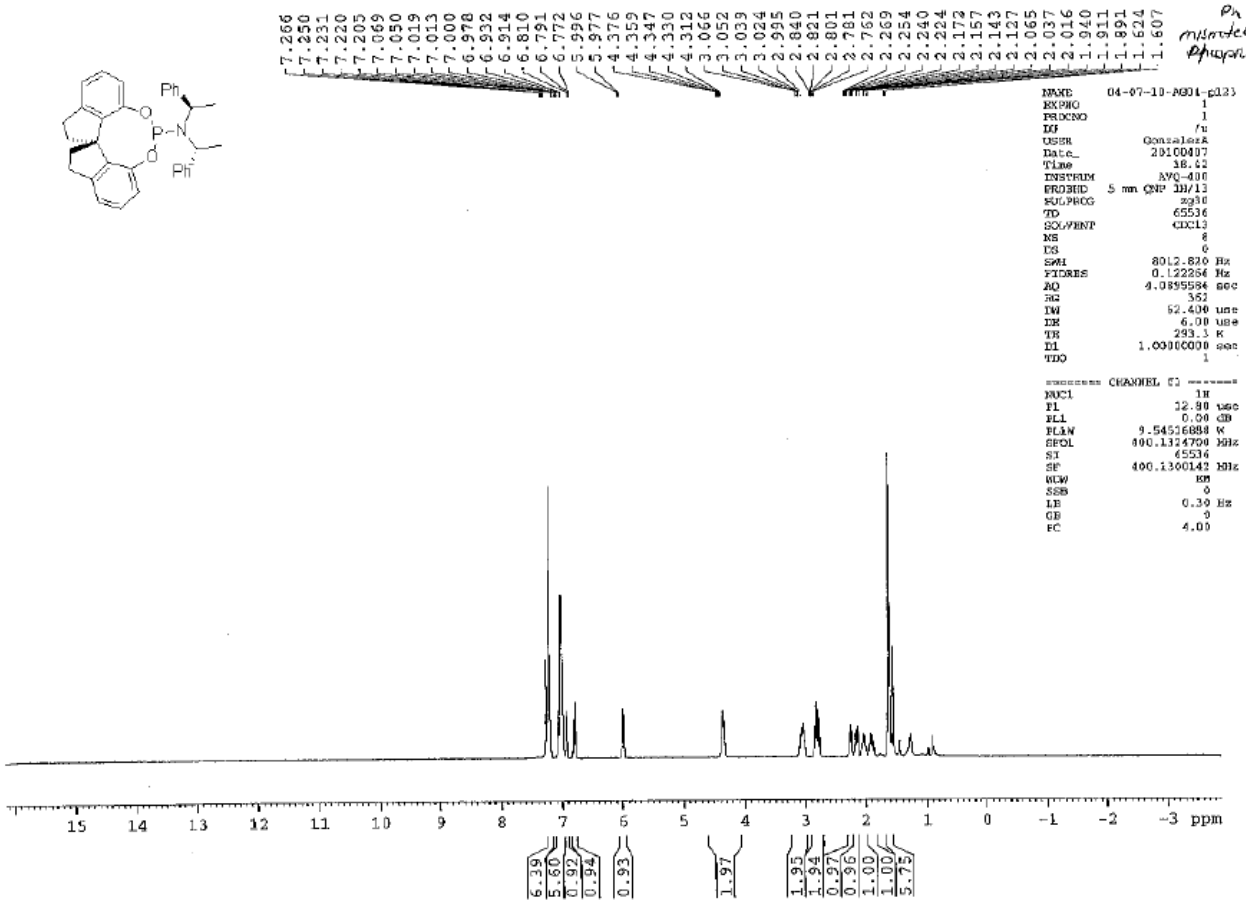
PL2 0.00 dB
PL12 14.22 dB
300 250 200 150 100 50 0 -50 -100 -150 -200 ppm

AVQ-400 loaner probe



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1.891
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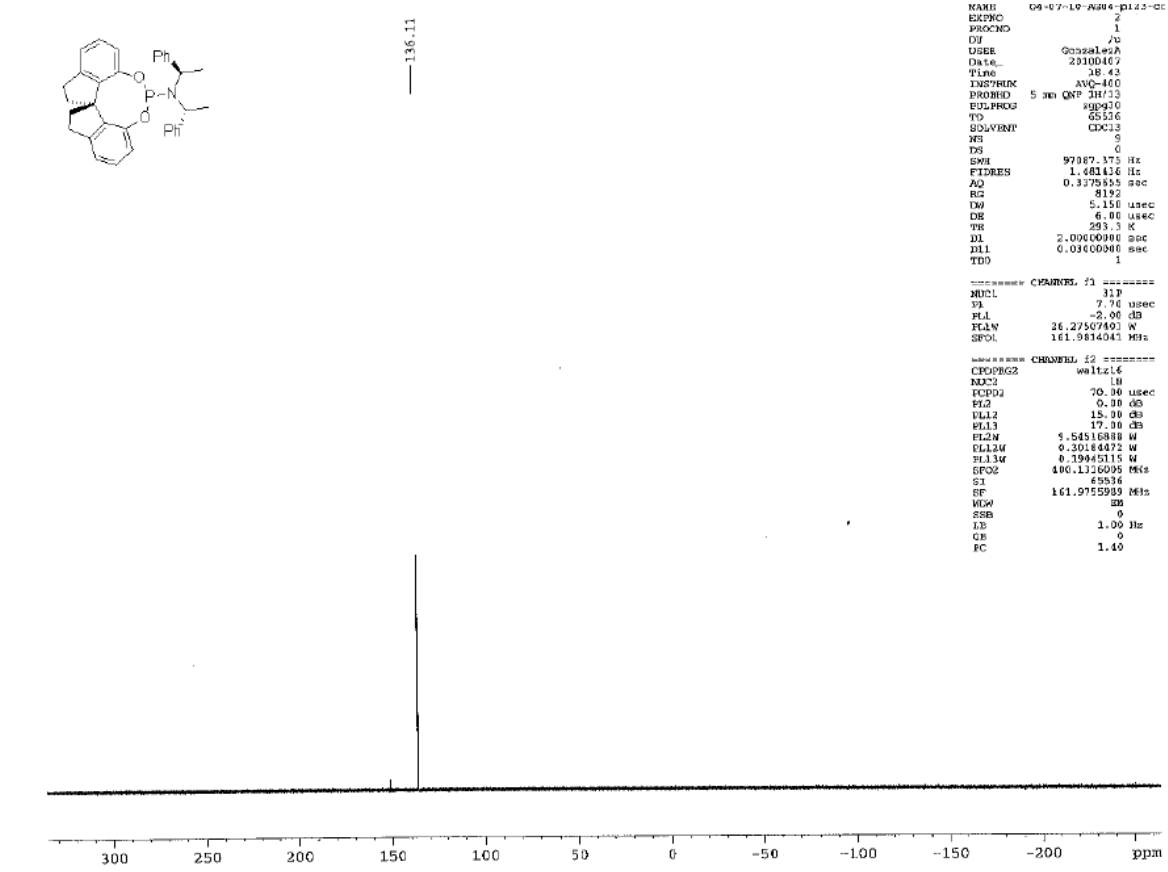
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O
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136.11
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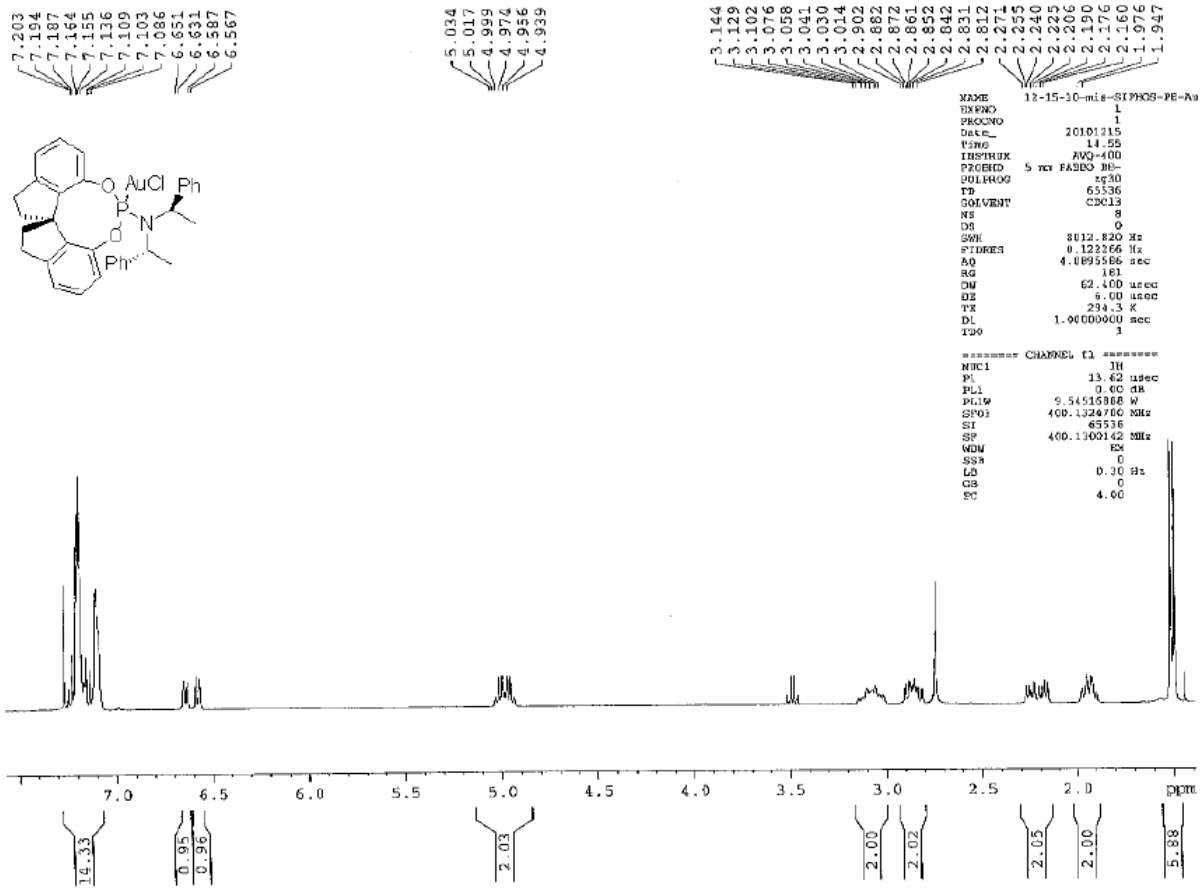
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P
N
O
Ph
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PROCNO 1
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PULPROG zg30
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SOLVENT CDCl3
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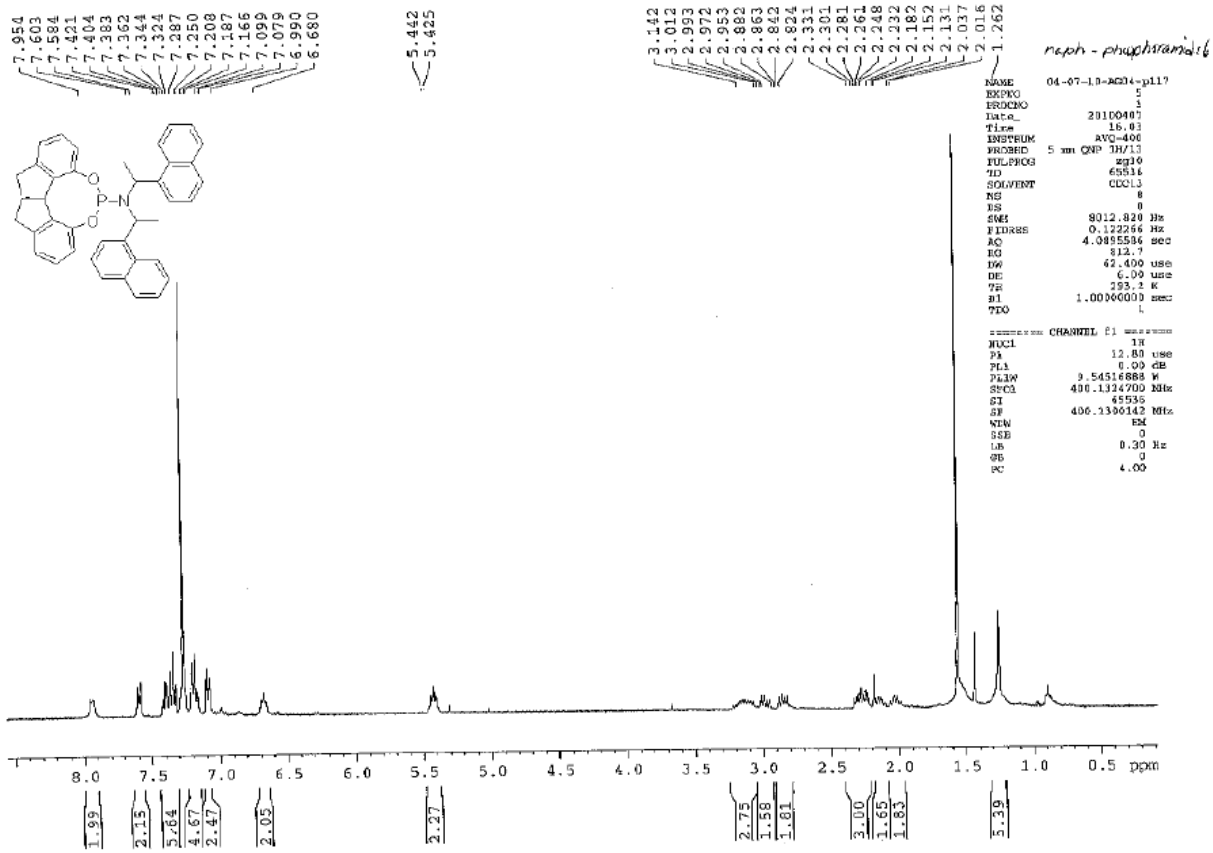
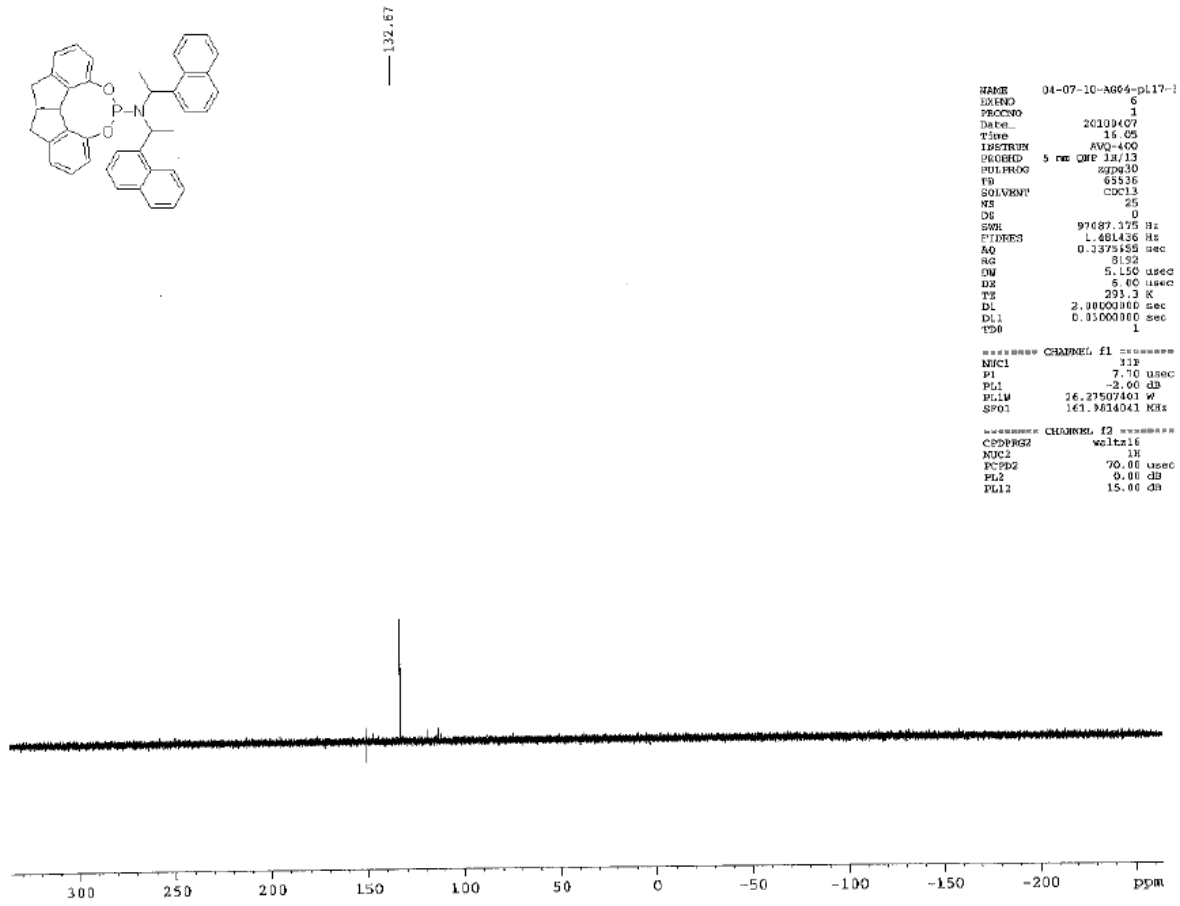
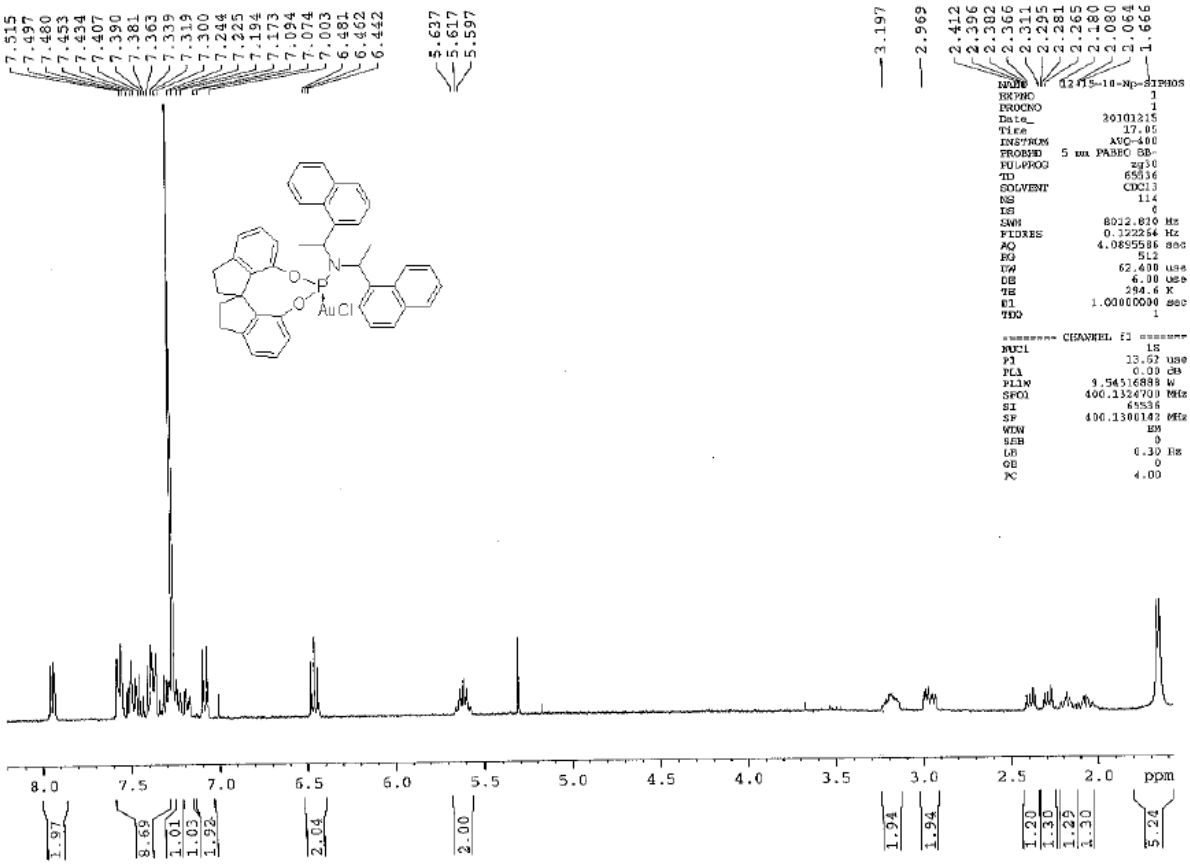
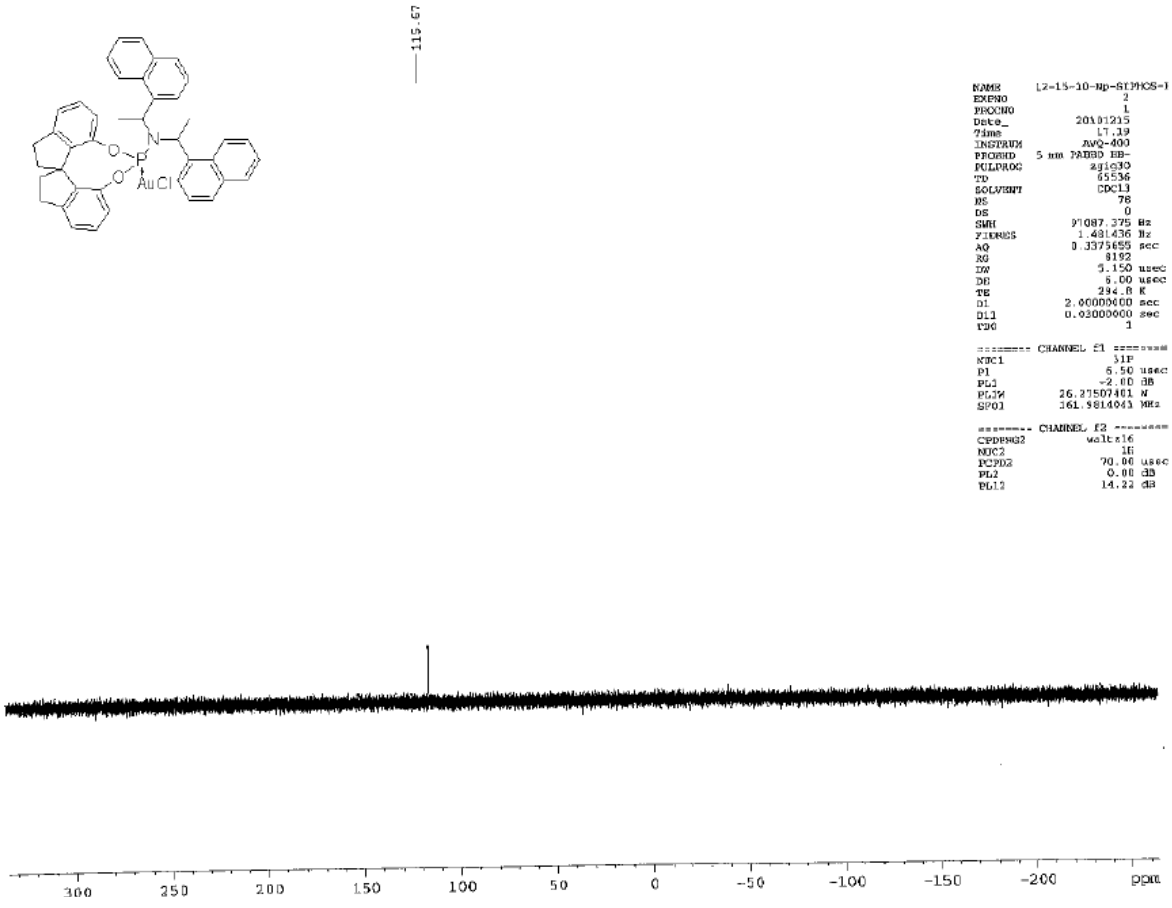
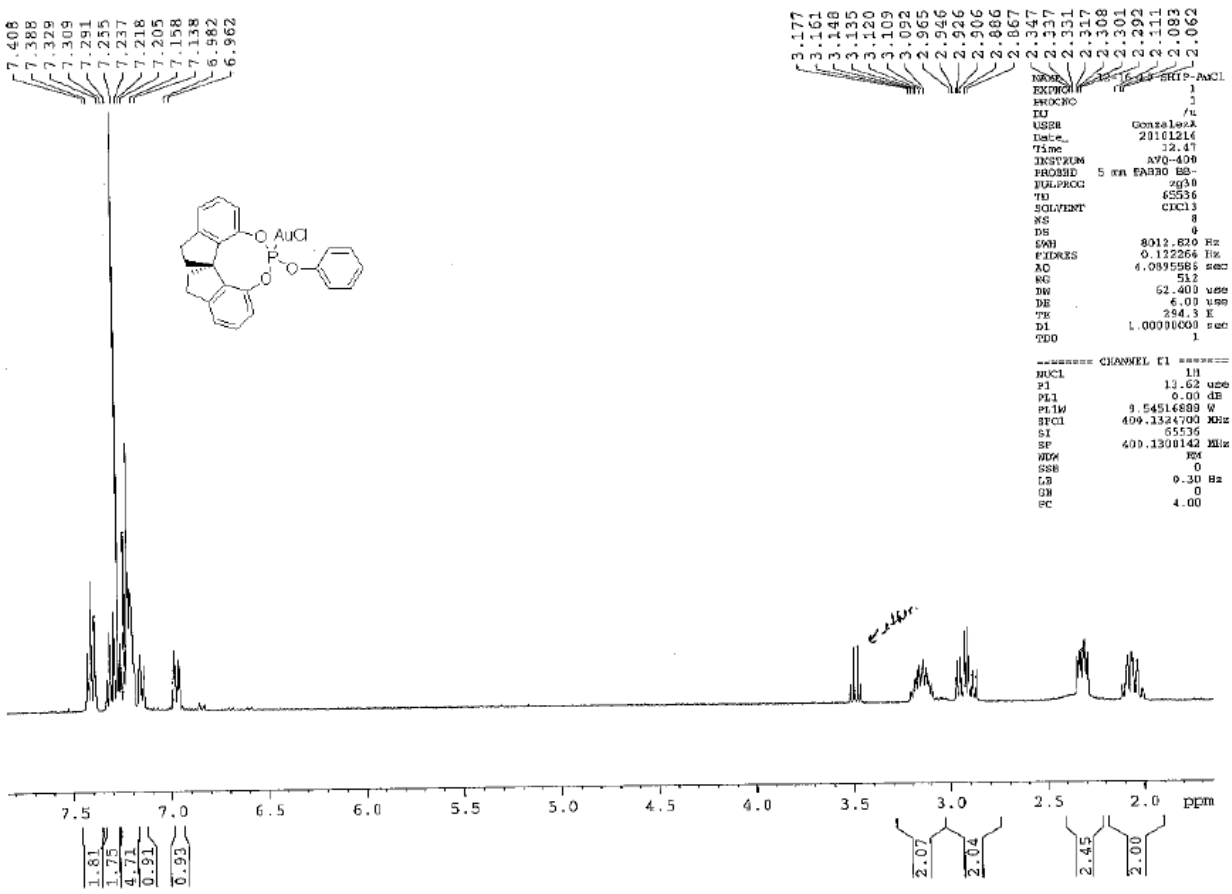
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 161
DW 62.400 usec
DE 6.00 usec
TE 294.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.62 usec
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324709 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
ppm
14.33
0.95
0.96
2.03
2.00
2.02
2.05
2.00
5.88
118.34
O AuCl Ph
P
N
O
Ph
NAME 12-15-10-mis-SIPHOS-
EXPNO 2
PROCNO 1
Date_ 20101215
Time 14.57
INSTRUM AVQ-400
PROBHD 5 mm PABBO BB-
PULPROG zgig30
TD 65536
SOLVENT CDCl3
NS 15
DS 0
SWH 97087.375 Hz
FIDRES 1.481436 Hz
AQ 0.1375655 sec
RG 8192
DW 5.150 usec
DE 6.00 usec
TE 294.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 31P
P1 6.50 usec
PL1 -2.00 dB
PL1W 26.29507401 W
SFO1 161.9814041 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 0.00 dB
PL12 14.22 dB
300
250
200
150
100
50
0
-50
-100
-150
-200
ppm

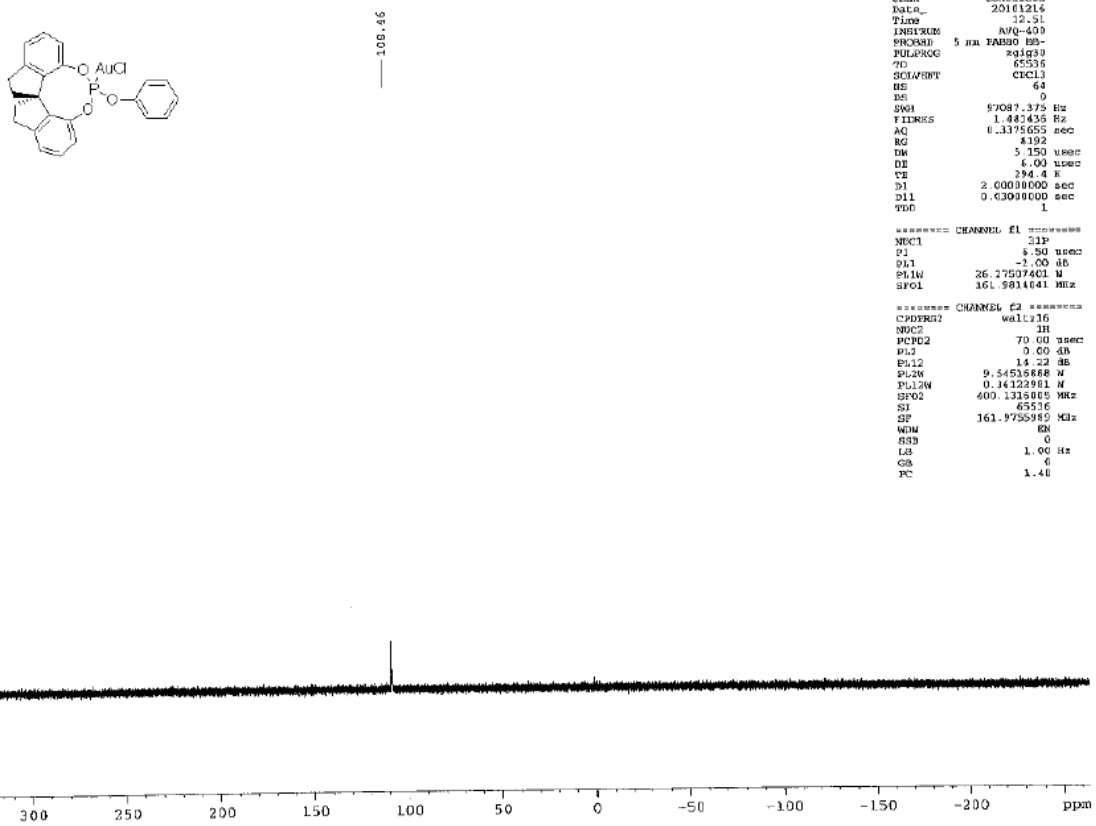

7.954
7.603
7.584
7.421
7.404
7.383
7.362
7.344
7.324
7.287
7.250
7.208
7.187
7.166
7.099
7.079
6.990
6.680
5.442
5.425
3.142
3.012
2.993
2.972
2.953
2.882
2.863
2.842
2.824
2.331
2.301
2.281
2.261
2.248
2.232
2.182
2.152
2.131
2.037
2.016
1.262
neph - phosphoramidite
NAME 04-07-10-AG04-p117
EXPNO 5
PROCNO 1
Date_ 20100407
Time 16.03
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0855536 sec
RG 812.7
DW 62.400 usec
DE 6.00 usec
TE 293.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 usec
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.99
2.15
5.64
4.67
2.47
2.05
2.27
2.75
1.58
1.81
3.00
1.65
1.83
5.39

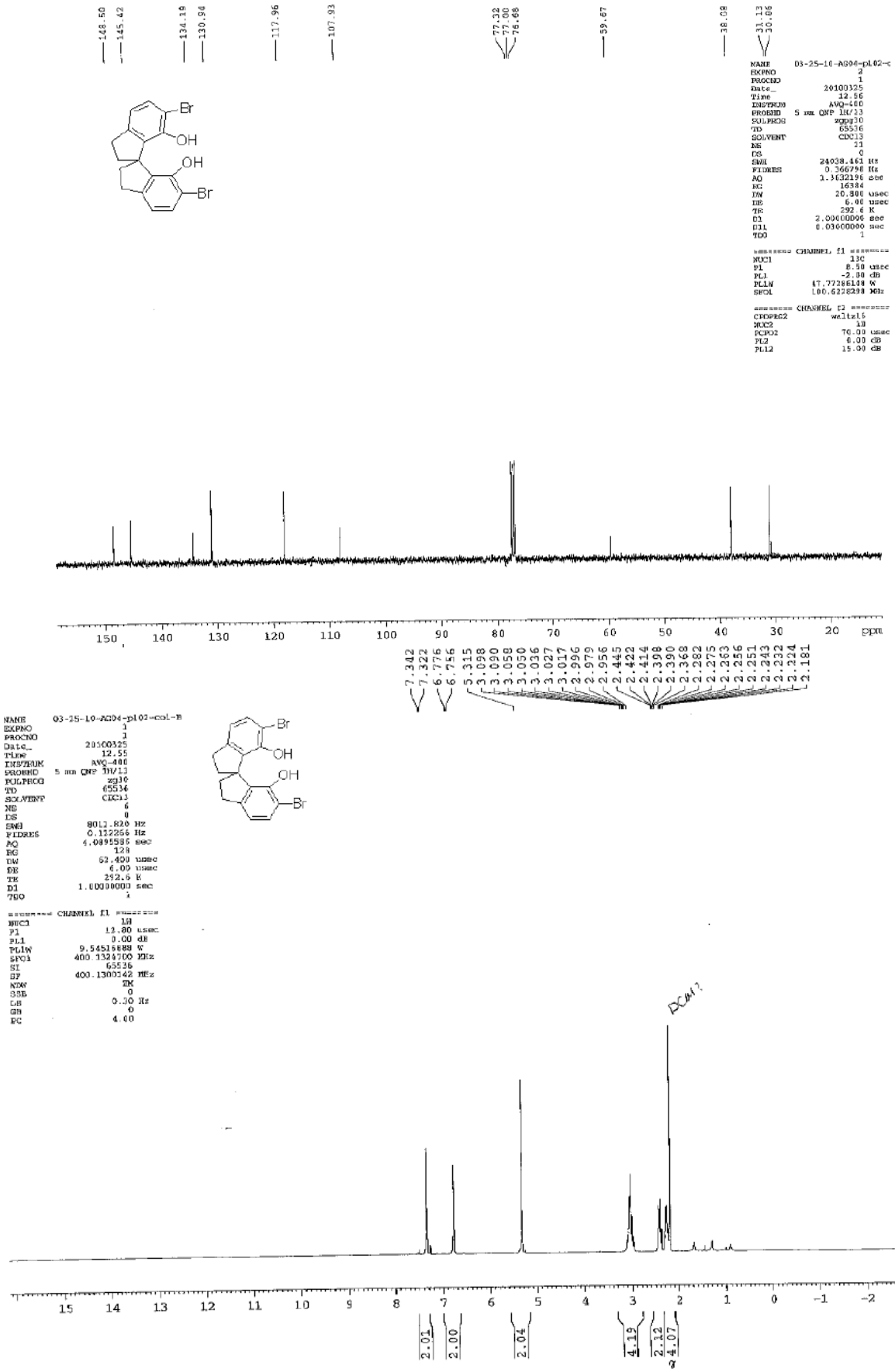

132.67
NAME 04-07-10-AG04-p117-1
EXPNO 6
PROCNO 1
Date_ 20100407
Time 16.05
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 25
DS 0
SWH 97087.375 Hz
FIDRES 1.481436 Hz
AQ 0.3375455 sec
RG 8192
DW 5.150 usec
DE 6.00 usec
TE 293.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 31P
P1 7.70 usec
PL1 -2.00 dB
PL1W 26.27507401 W
SFO1 161.9814041 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 0.00 dB
PL12 15.00 dB
300 250 200 150 100 50 0 -50 -100 -150 -200 ppm

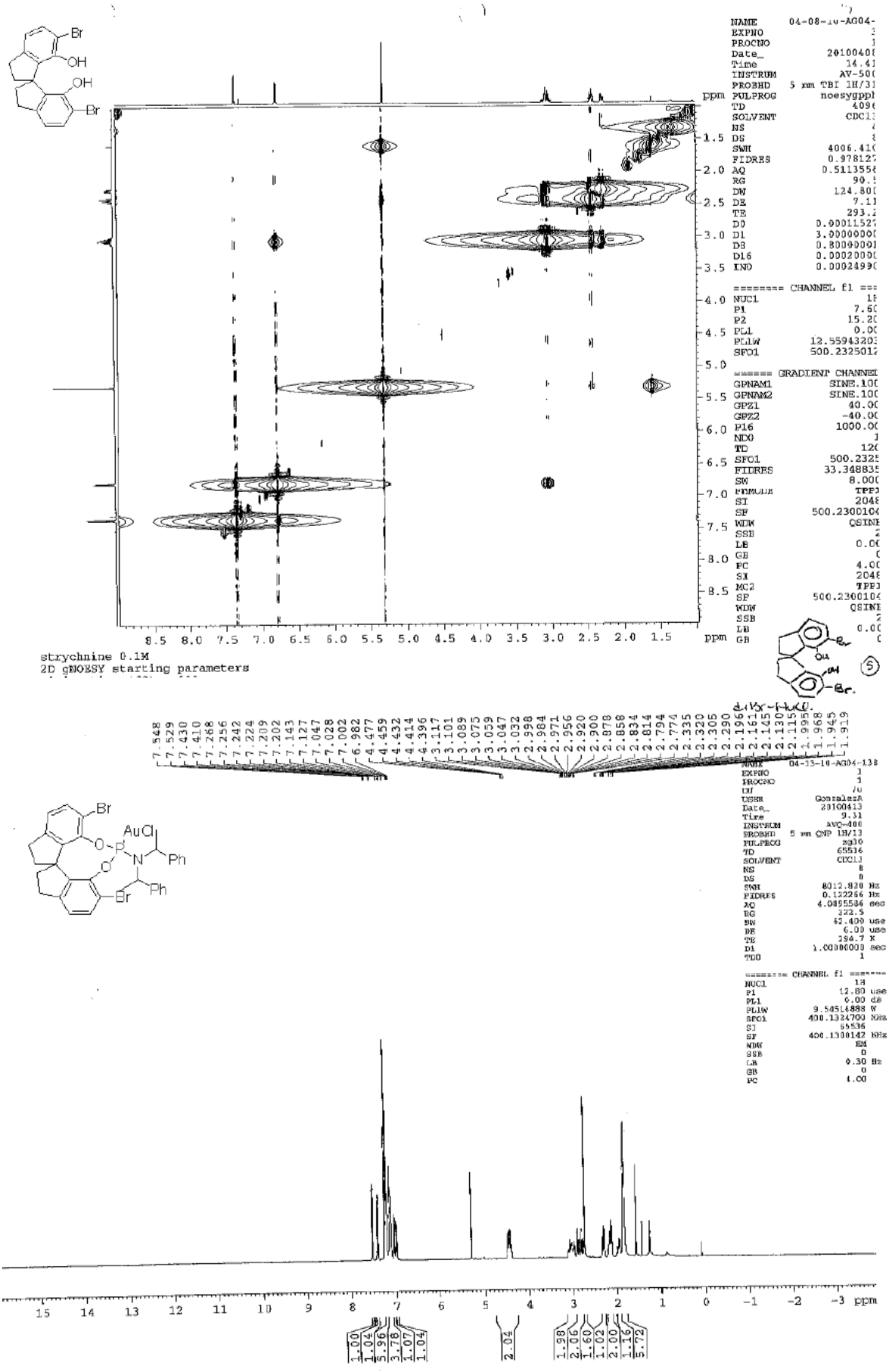

7.515
7.497
7.480
7.453
7.434
7.407
7.390
7.381
7.363
7.339
7.319
7.300
7.244
7.225
7.194
7.173
7.094
7.074
7.003
6.481
6.462
6.442
5.637
5.617
5.597
3.197
2.969
2.412
2.396
2.382
2.366
2.311
2.295
2.281
2.265
2.180
2.080
2.064
1.666
Au Cl
NAME L2-15-10-Np-SIPHOS
EXPNO 1
PROCNO 1
Date_ 20101215
Time 17.05
INSTRUM AVQ-400
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 114
DS 6
SWH 8012.820 Hz
FIDRES 0.122264 Hz
AQ 4.0895586 sec
RG 512
DW 62.400 usec
DE 6.00 usec
TE 294.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.62 usec
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324709 MHz
SI 65536
SF 400.1300148 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
ppm
1.97
8.69
1.01
1.03
1.92
2.04
2.00
1.94
1.94
1.20
1.30
1.29
3.30
5.24


115.67
Au Cl
NAME L2-15-10-Np-SIPHOS-1
EXPNO 2
PROCNO 1
Date_ 20101215
Time 17.19
INSTRUM AVQ-400
PROBHD 5 mm PABBO BB-
PULPROG zgig30
TD 65536
SOLVENT CDCl3
NS 78
DS 0
SWH 81087.375 Hz
FIDRES 1.481436 Hz
AQ 0.8375655 sec
RG 8192
DW 5.150 usec
DE 6.00 usec
TE 294.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 31P
P1 6.50 usec
PL1 -2.00 dB
PL1W 26.27507401 W
SFO1 161.9814043 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 0.00 dB
PL12 14.22 dB
300
250
200
150
100
50
0
-50
-100
-150
-200
ppm

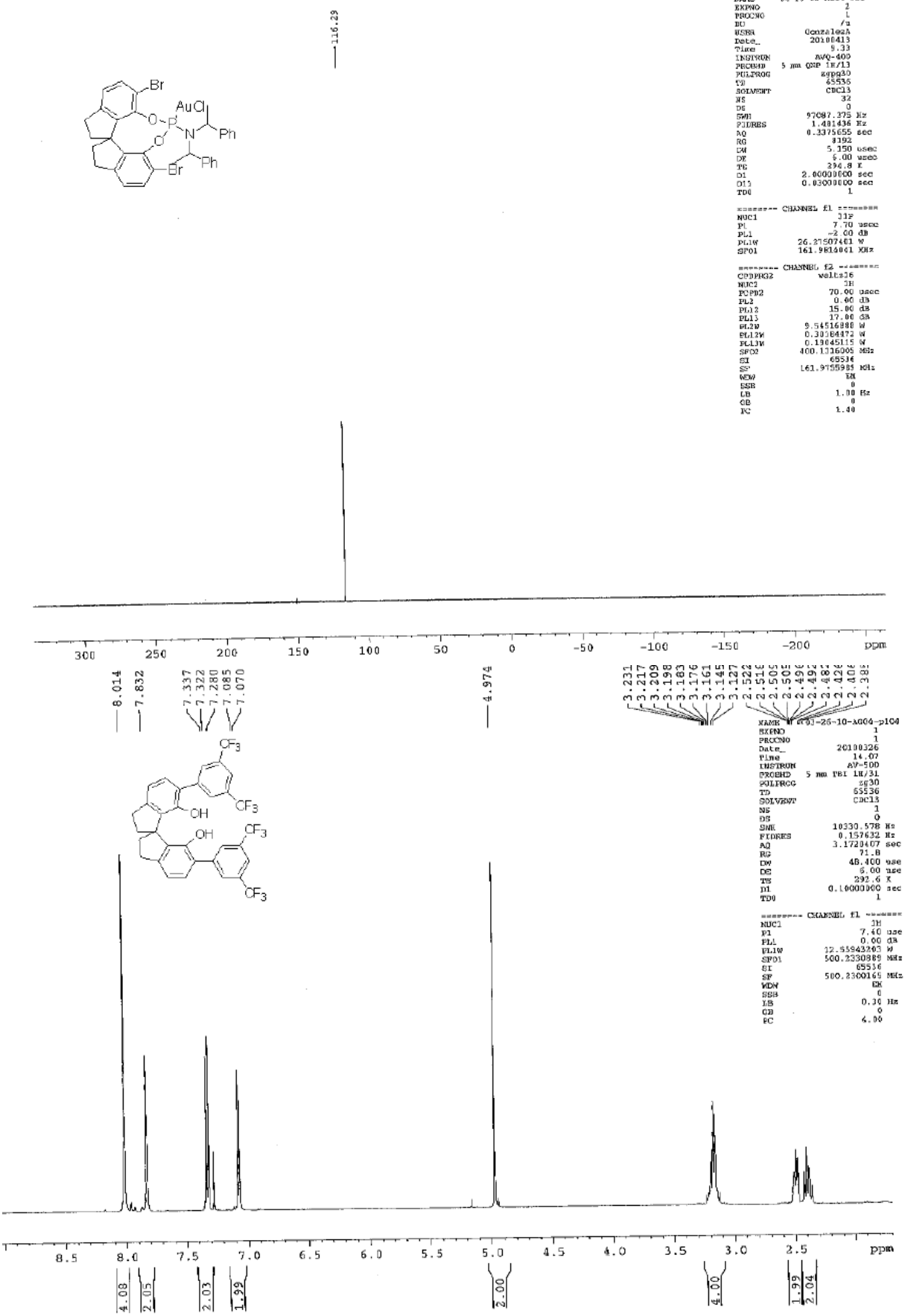

7.408
7.388
7.329
7.309
7.291
7.255
7.237
7.218
7.205
7.158
7.138
6.982
6.962
3.177
3.161
3.148
3.135
3.120
3.109
3.092
2.965
2.946
2.926
2.906
2.886
2.867
2.347
2.331
2.317
2.308
2.301
2.292
2.111
2.083
2.062
O AuCl
P
O
O
NAME 12-16-10-SHIP-AuCl
EXPNO 1
PROCNO 1
DU /u
USER GonzalezA
Date_ 20101216
Time 12.47
INSTRUM AVQ-400
PROBHD 5 mm BBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122264 Hz
AQ 4.0895565 sec
RG 512
DW 62.400 usec
DE 6.00 usec
TE 294.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.62 usec
PL1 0.00 dB
PL1W 9.54514888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
ppm
1.81
1.75
4.71
0.91
0.93
2.07
2.04
2.45
2.00

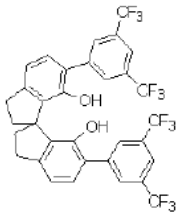

O AuCl
P
O
O
108.46
NAME 12-16-10-SHIP-AuCl
EXPNO 2
PROCNO 1
DU /u
USER GonzalezA
Date_ 20101216
Time 12.51
INSTRUM AVQ-400
PROBHD 5 mm BBO BB-
PULPROG zgig30
TD 65536
SOLVENT CDCl3
NS 64
DS 0
SWH 97087.375 Hz
FIDRES 1.482436 Hz
AQ 0.3375655 sec
RG 8192
DW 5.150 usec
DE 6.00 usec
TE 294.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 31P
P1 6.50 usec
PL1 -2.00 dB
PL1W 26.27507401 W
SFO1 161.9814041 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 0.00 dB
PL12 14.22 dB
PL2W 9.54514888 W
PL12W 0.14122981 W
SFO2 400.1316005 MHz
SI 65536
SF 161.9755989 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
300
250
200
150
100
50
0
-50
-100
-150
-200
ppm


148.50
145.42
134.19
130.94
117.96
107.93
77.32
77.00
76.68
59.67
38.08
31.13
30.86
Br
OH
OH
Br
NAME 03-25-10-AG04-pl02-c
EXPNO 2
PROCNO 1
Date_ 20100325
Time 12.55
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 21
DS 0
SWH 24038.461 Hz
FIDRES 0.366796 Hz
AQ 1.3632196 sec
RG 16384
DW 20.800 usec
DE 6.00 usec
TE 292.6 K
D1 2.00000006 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 -2.00 dB
PL1W 47.77286148 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 0.00 dB
PL12 15.00 dB
150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm
7.342
7.322
6.776
6.756
5.315
3.098
3.090
3.058
3.050
3.036
3.027
3.017
2.996
2.979
2.956
2.445
2.422
2.414
2.398
2.390
2.368
2.282
2.275
2.263
2.256
2.251
2.243
2.232
2.224
2.181
NAME 03-25-10-AG04-pl02-col-B
EXPNO 1
PROCNO 1
Date_ 20100325
Time 12.55
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8012.820 Hz
FIDRES 0.122256 Hz
AQ 4.0895586 sec
RG 128
DW 62.400 usec
DE 6.00 usec
TE 292.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.80 usec
PL1 0.00 dB
PL1W 9.54515888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
Br
OH
OH
Br
DCM?
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 ppm
2.01
2.00
2.04
4.19
2.12
4.07

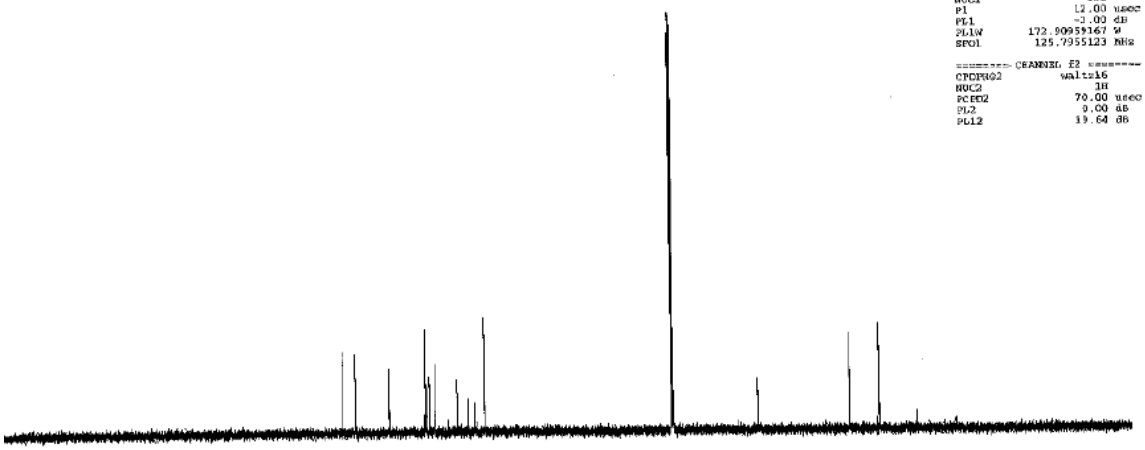

strychnine 0.1M
2D gNOESY starting parameters

Br
AuCl
O
P
O
N
Ph
Ph
Br

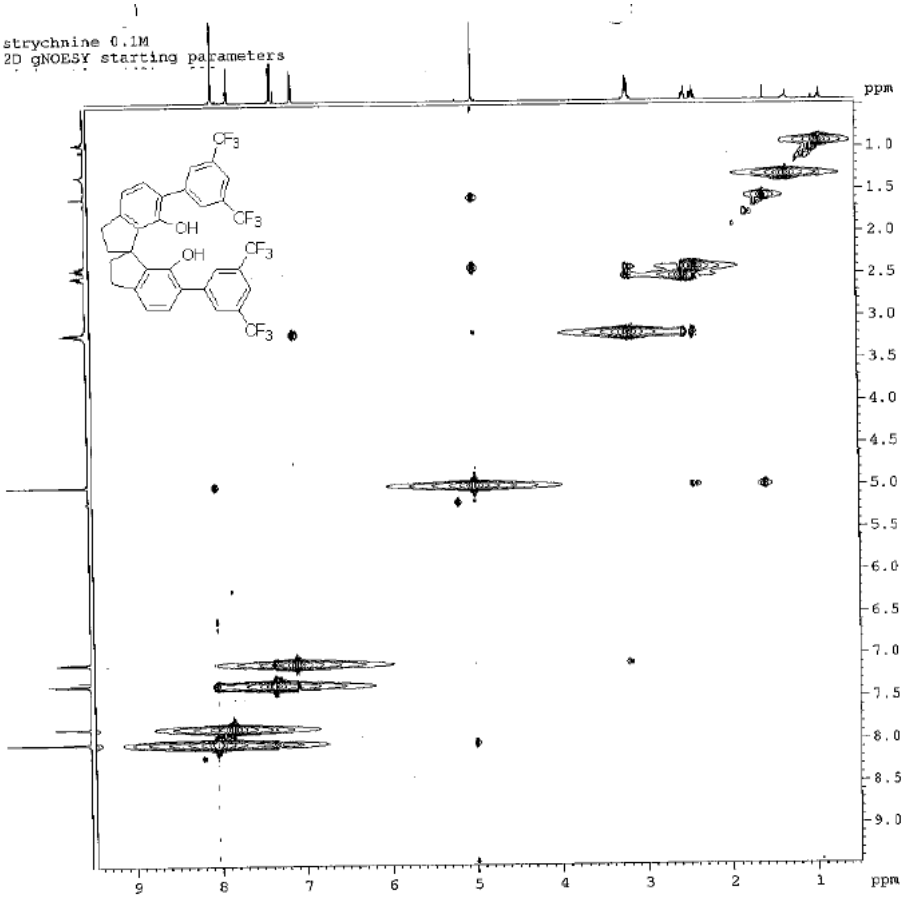

116.29
NAME 04-13-10-AG04-138
EXPNO 2
PROCNO 1
USER GonzalezA
Date_ 20100413
Time 9.33
INSTRUM AVQ-400
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 97087.375 Hz
FIDRES 1.481436 Hz
AQ 0.3375655 sec
RG 8192
DW 5.150 usec
DE 6.00 usec
TE 294.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
NUC1 31P
P1 7.70 usec
PL1 -2.00 dB
PL1W 26.21507401 W
SFO1 161.9814041 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 17.00 dB
PL2W 9.54516888 W
PL12W 0.30384472 W
PL13W 0.19045115 W
SFO2 400.1316005 MHz
SI 65536
SF 161.9755985 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
300 250 200 150 100 50 0 -50 -100 -150 -200 ppm
8.014 7.832 7.337 7.322 7.280 7.085 7.070 4.974
3.231 3.217 3.209 3.198 3.183 3.176 3.161 3.145 3.127 2.522 2.515 2.505 2.498 2.492 2.484 2.424 2.408 2.383
CF3
CF3
OH
OH
CF3
CF3
NAME 04-26-10-AG04-p104
EXPNO 1
PROCNO 1
Date_ 20100326
Time 14.07
INSTRUM AV-500
PROBHD 5 mm TBI 1H/31
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 71.8
DW 48.400 usec
DE 6.00 usec
TE 292.6 K
D1 0.10000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 7.40 usec
PL1 0.00 dB
PL1W 12.55943203 W
SFO1 500.2330889 MHz
SI 65536
SF 500.2300169 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 ppm
4.08 2.05 2.03 1.99 2.00 4.00 1.99 2.04

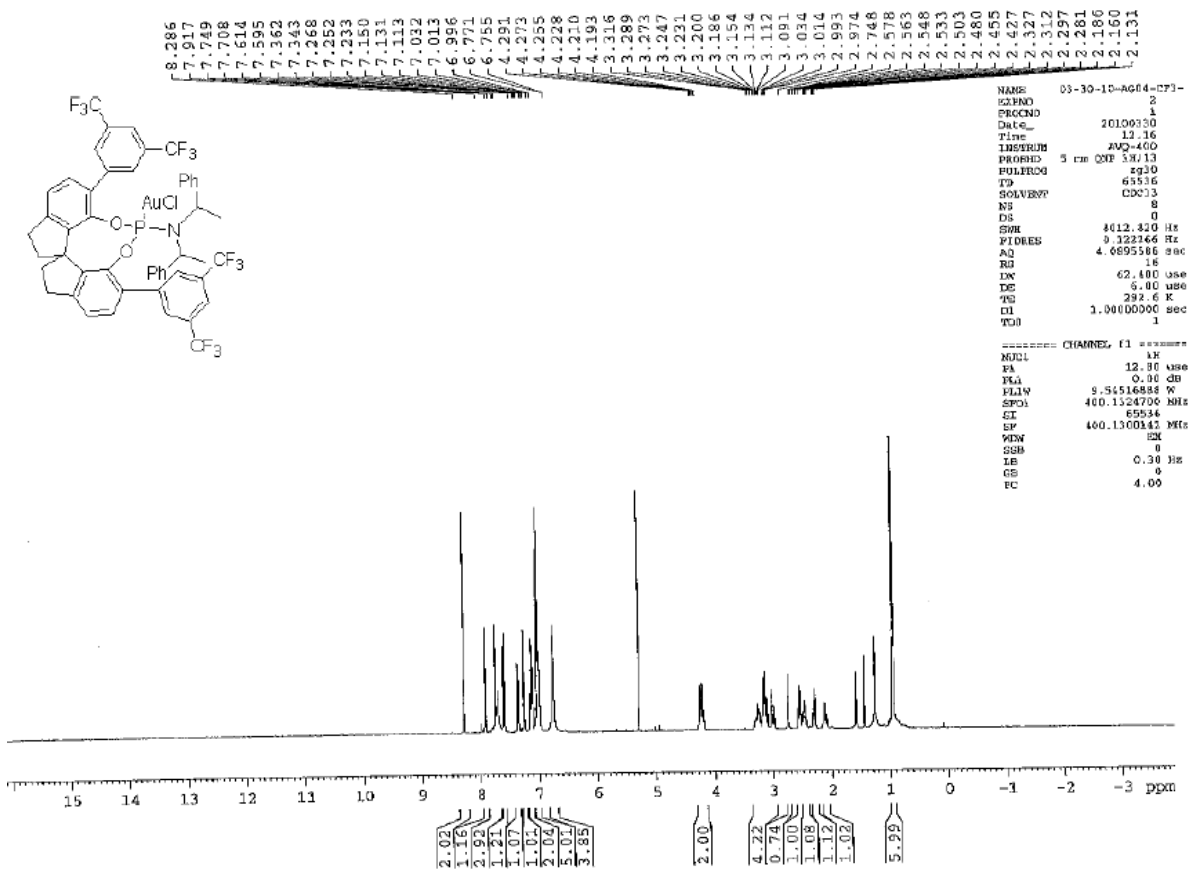


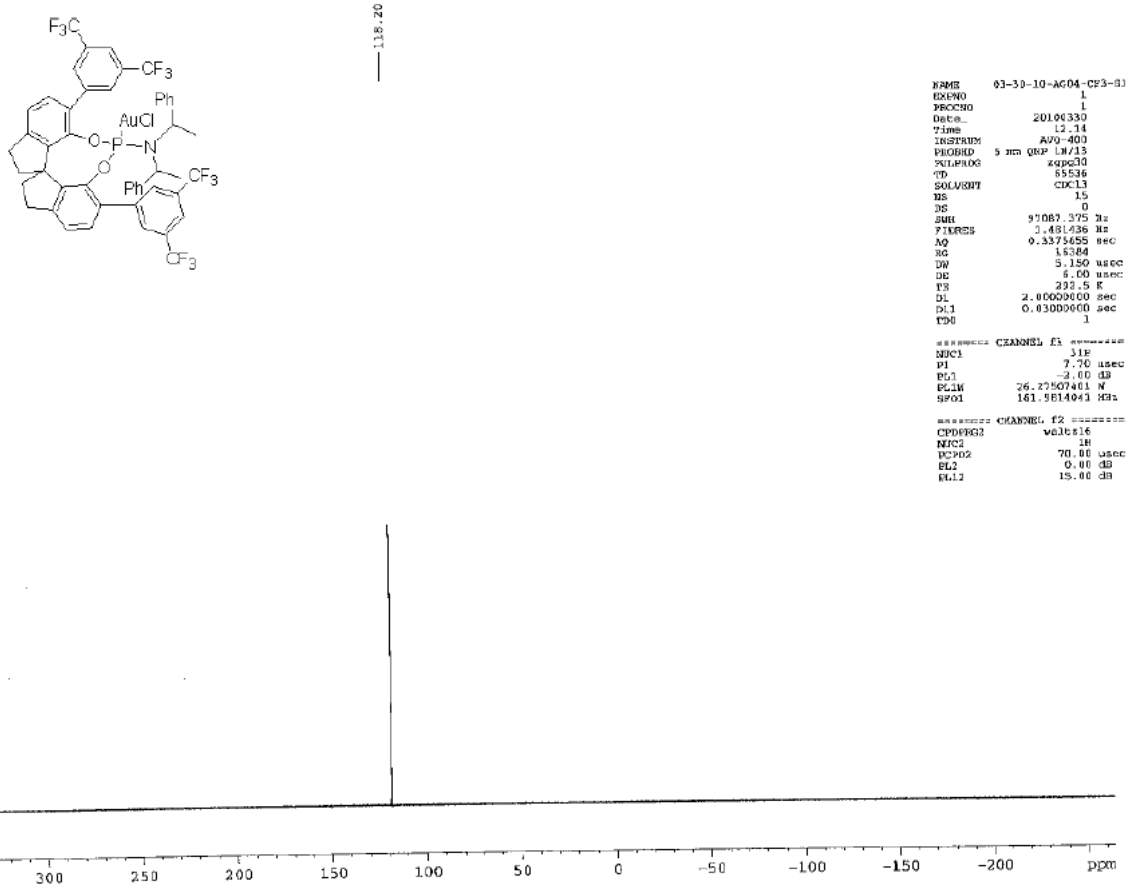
149.80
147.04
139.60
131.63
131.38
131.32
130.62
129.59
129.49
124.46
123.30
118.58
77.25
77.00
76.75
57.88
37.62
31.14

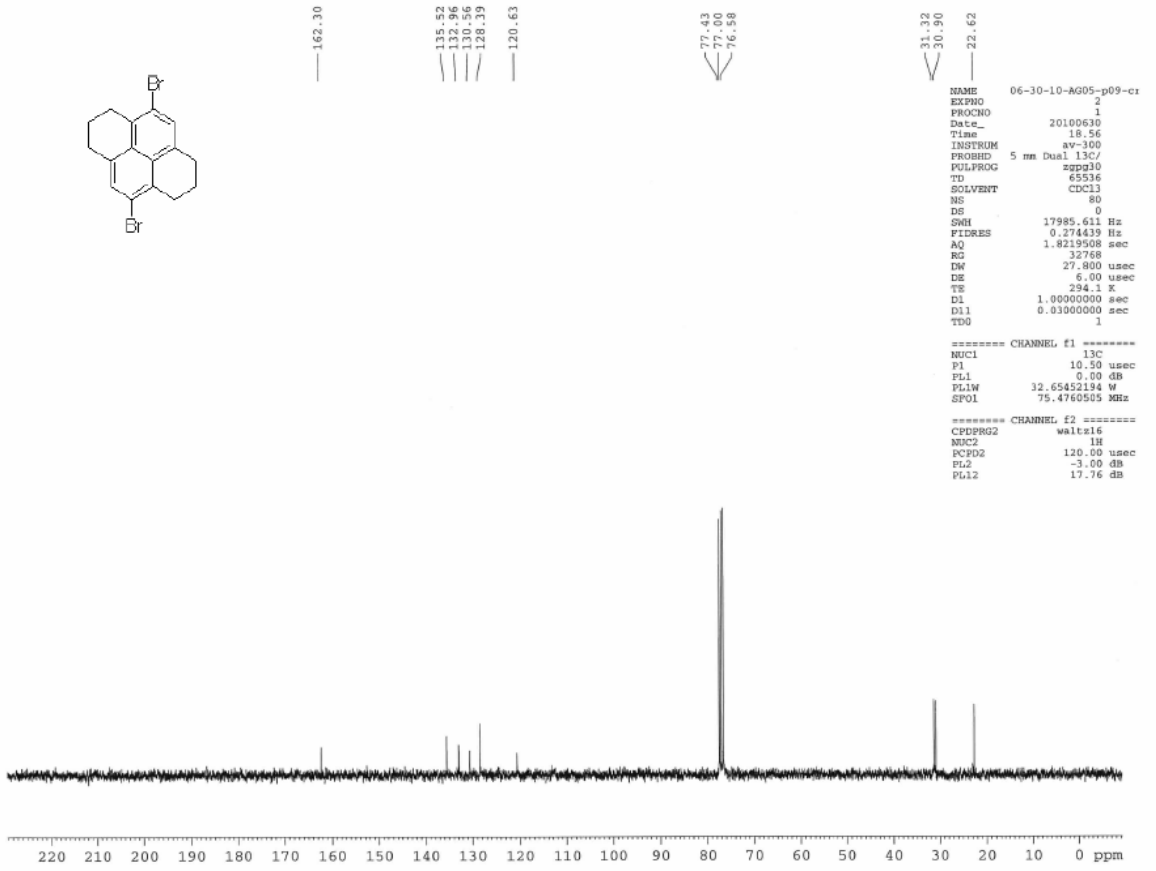


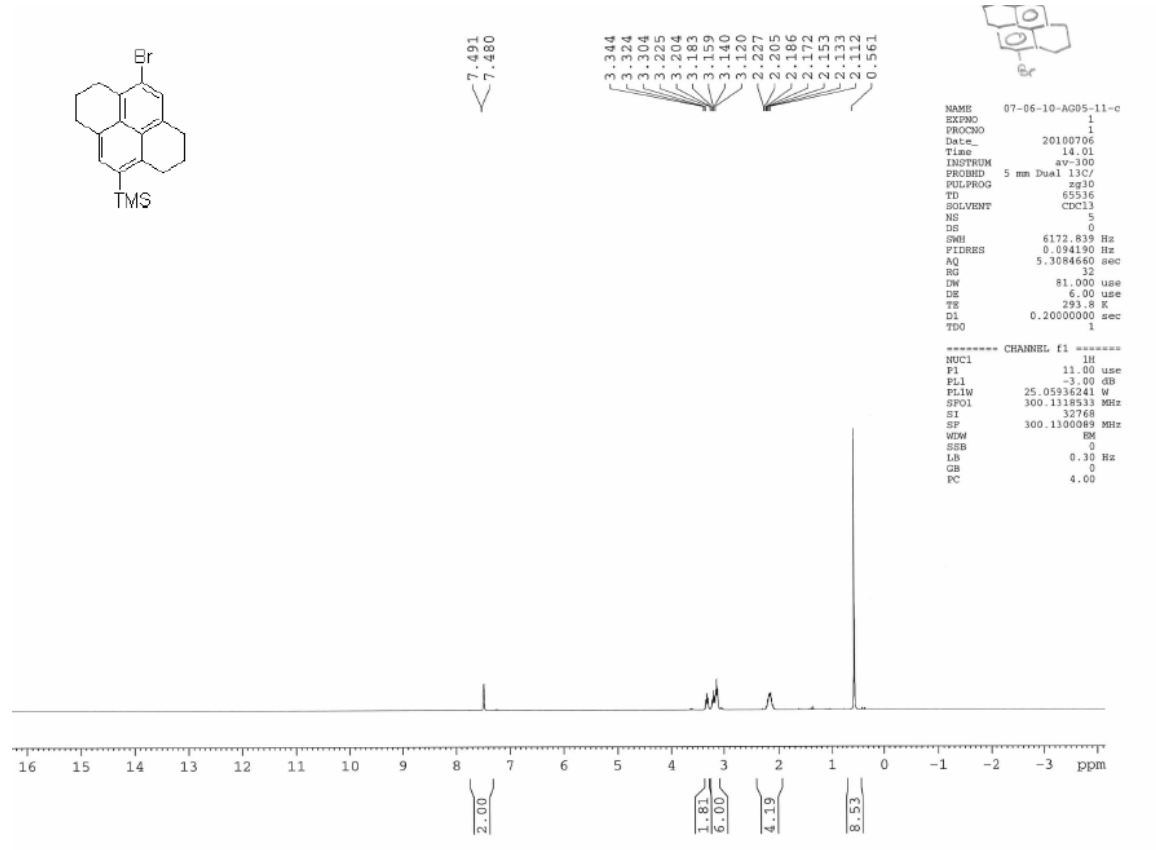
strychnine 0.1M
2D gNOESY starting parameters

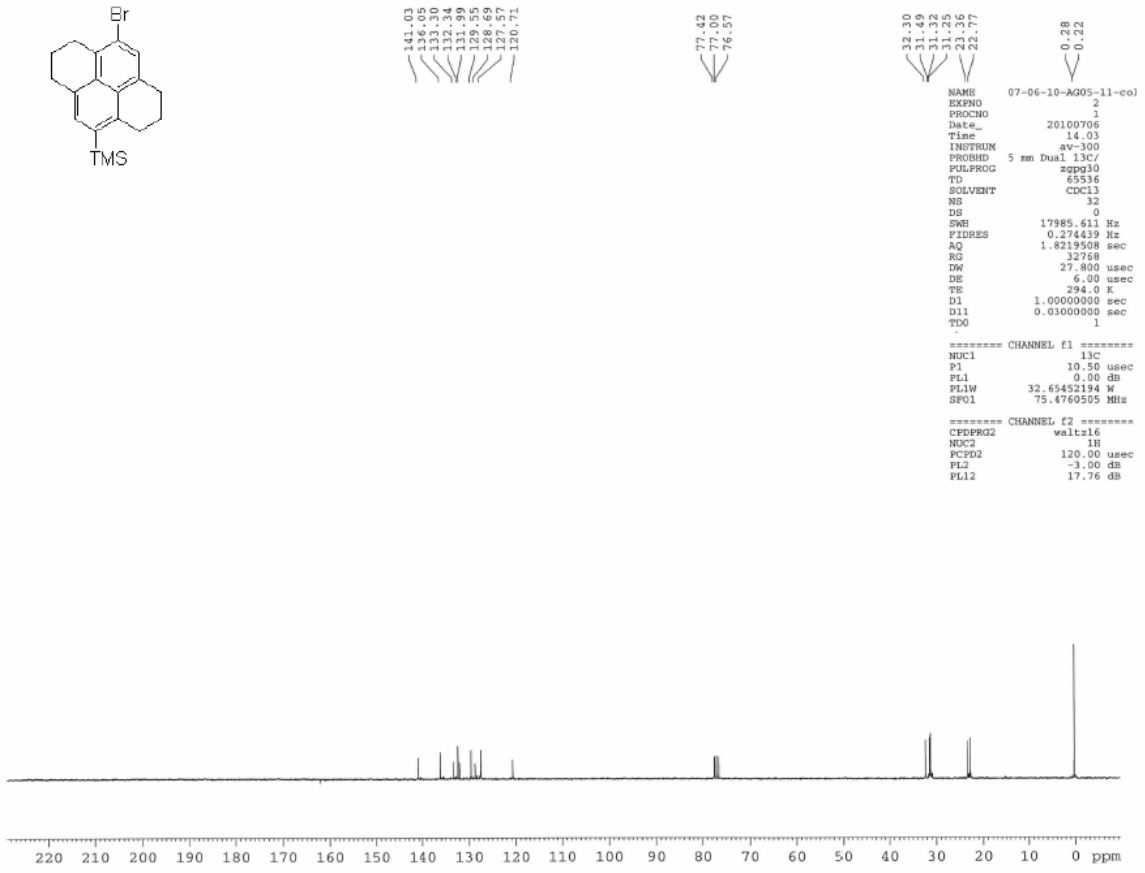


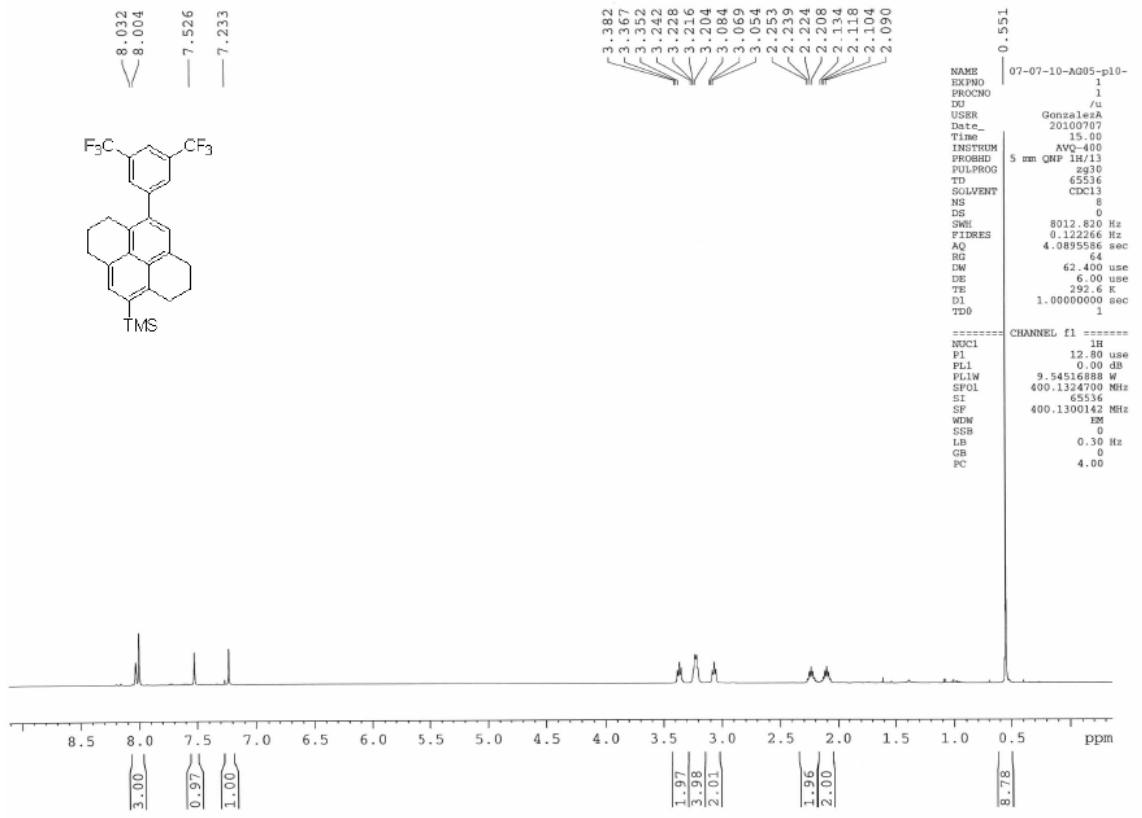

8.286
7.917
7.749
7.708
7.614
7.595
7.362
7.343
7.268
7.252
7.233
7.150
7.131
7.113
7.032
7.013
6.996
6.771
6.755
4.291
4.273
4.255
4.228
4.210
4.193
3.316
3.289
3.273
3.247
3.231
3.200
3.186
3.154
3.134
3.112
3.091
3.034
3.014
2.993
2.974
2.748
2.578
2.563
2.548
2.533
2.503
2.480
2.455
2.427
2.327
2.312
2.297
2.281
2.186
2.160
2.131
F3C
CF3
Ph
AuCl
O-P-N
O
Ph
CF3
CF3
NAME 03-30-10-AG04-CF3-
EXPNO 2
PROCNO 1
Date_ 20100330
Time 12.16
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 16
DW 62.400 usec
DE 6.00 usec
TE 292.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 usec
PL1 0.00 dB
PL1W 9.56516888 W
SFO1 400.1324706 MHz
SI 65536
SF 400.1300141 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 ppm
2.02
1.16
2.92
1.21
1.07
1.01
2.04
5.01
3.85
2.00
4.22
0.74
1.00
1.08
1.12
1.02
5.99

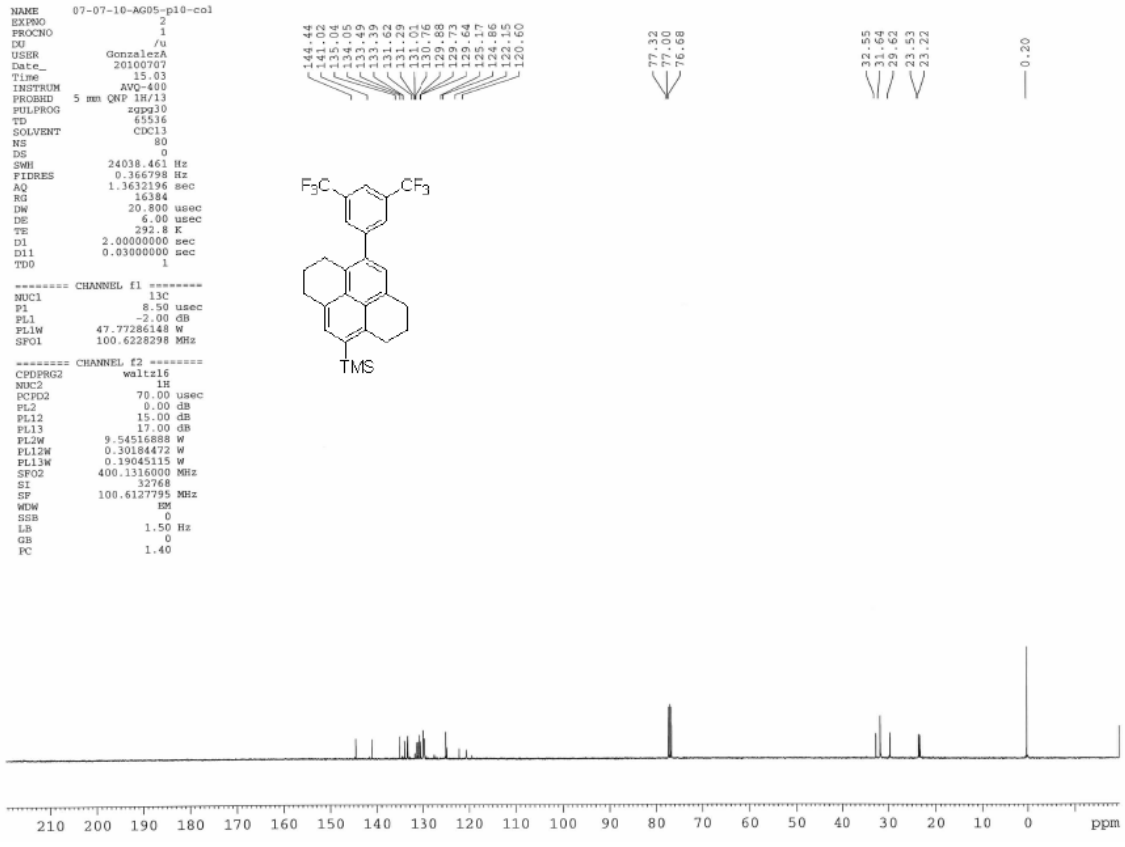

118.20
F3C
CF3
Ph
AuCl
O-P-N
O
Ph
CF3
CF3
NAME 03-30-10-AG04-CF3-31
EXPNO 1
PROCNO 1
Date_ 20100330
Time 12.14
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 15
DS 0
SWH 97087.375 Hz
FIDRES 1.481436 Hz
AQ 0.3375655 sec
RG 16384
DW 5.150 usec
DE 6.00 usec
TE 292.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 31P
P1 7.70 usec
PL1 -2.00 dB
PL1W 26.27507401 W
SFO1 161.9814043 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 0.00 dB
PL12 15.00 dB
300 250 200 150 100 50 0 -50 -100 -150 -200 ppm

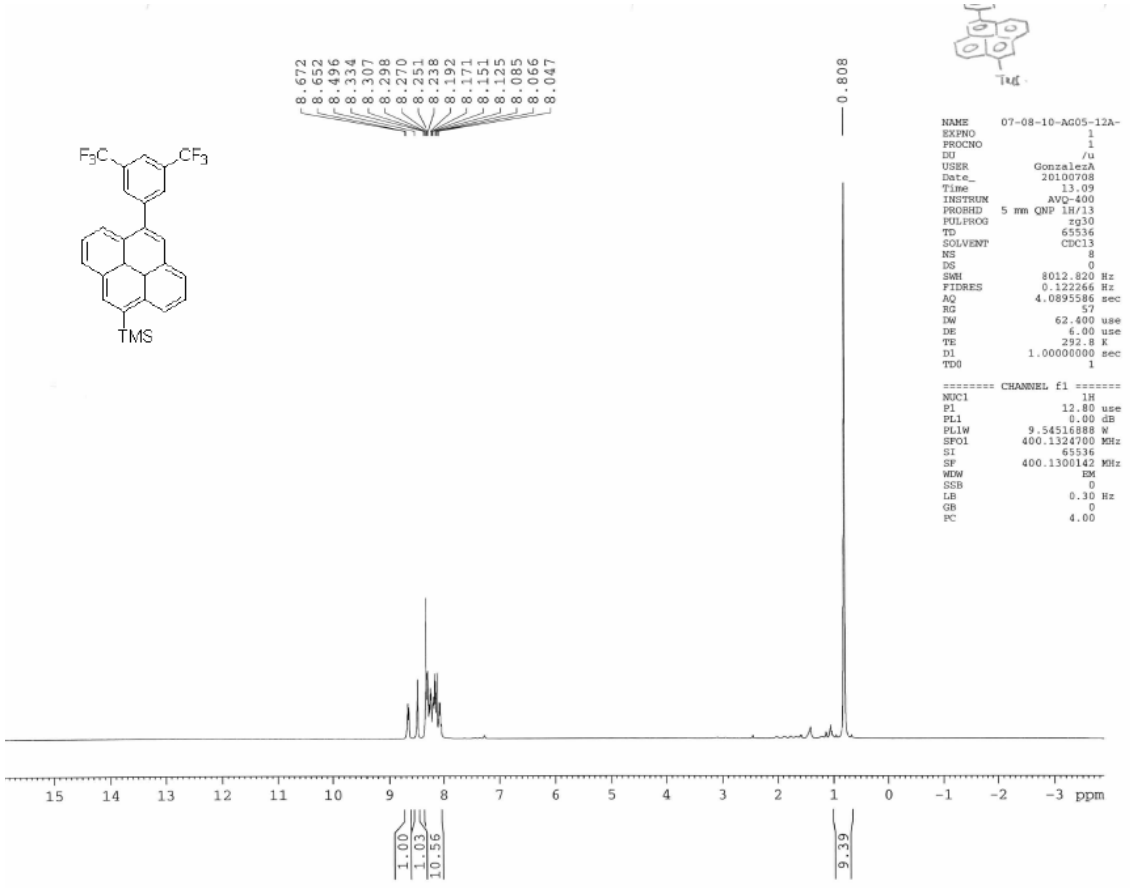

Br
Br
162.30
135.52
132.96
130.56
128.39
120.63
77.43
77.00
76.58
31.32
30.90
22.62
NAME 06-30-10-AG05-p09-c
EXPNO 2
PROCNO 1
Date_ 20100630
Time 18.56
INSTRUM av-300
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 80
DS 0
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 294.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 0.00 dB
PL1W 32.65452194 W
SFO1 75.4760505 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 120.00 usec
PL2 -3.00 dB
PL12 17.76 dB
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

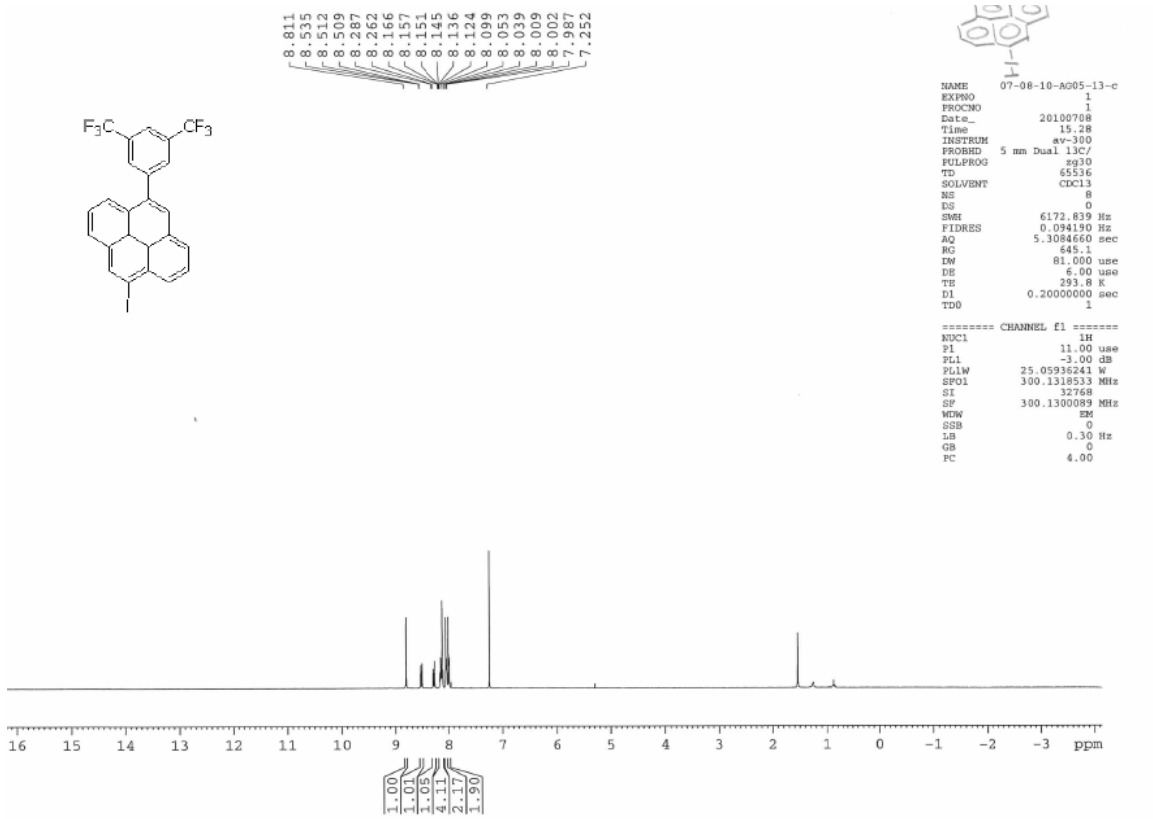

Br
TMS
7.491
7.480
3.344
3.324
3.304
3.225
3.204
3.183
3.159
3.140
3.120
2.227
2.205
2.186
2.172
2.153
2.133
2.112
0.561
NAME 07-06-10-AG05-11-c
EXPNO 1
PROCNO 1
Date_ 20100706
Time 14.01
INSTRUM av-300
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 5
DS 0
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 32
DW 81.000 use
DE 6.00 use
TE 293.8 K
D1 0.20000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.00 use
PL1 -3.00 dB
PL1W 25.05936241 W
SFO1 300.1318533 MHz
SI 32768
SF 300.1300089 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 ppm
2.00
1.81
6.00
4.19
8.53

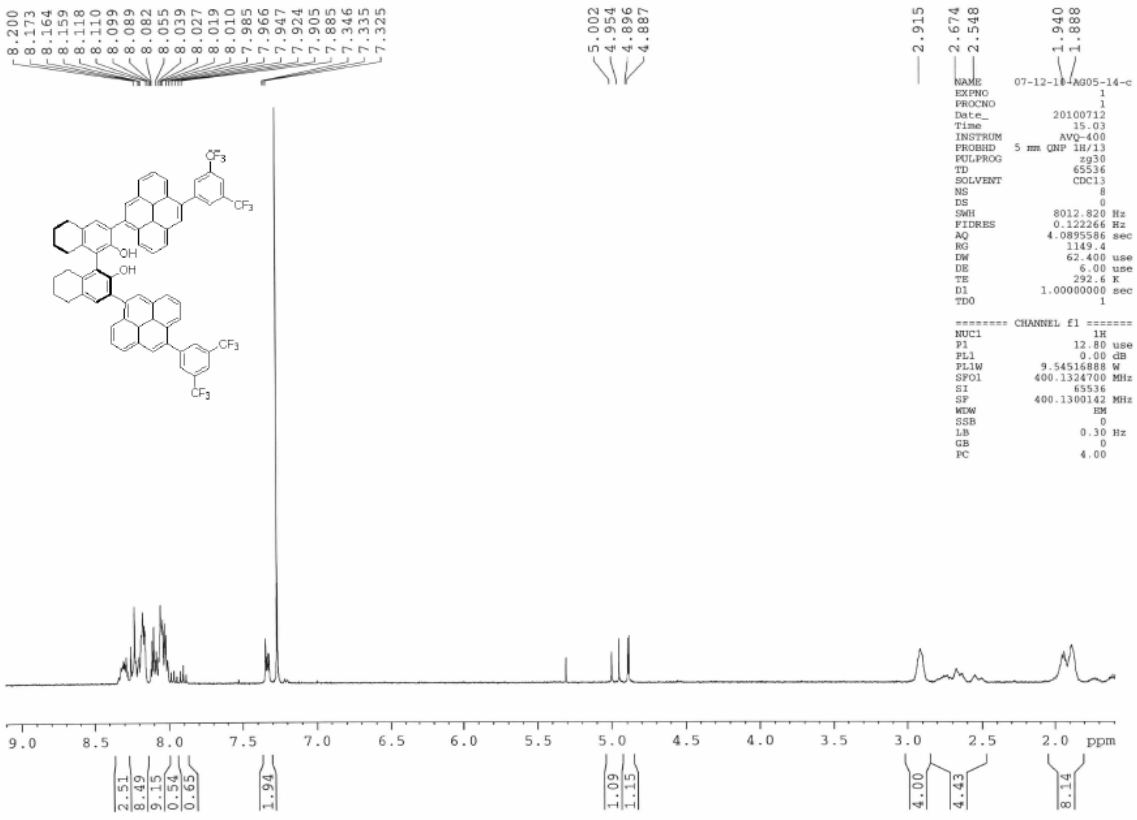

Br
TMS
141.03
136.05
133.30
132.34
131.99
129.55
128.69
127.57
120.71
77.42
77.00
76.57
32.30
31.49
31.42
31.25
23.36
22.77
0.28
0.22
NAME 07-06-10-AG05-11-col
EXPNO 2
PROCNO 1
Date_ 20100706
Time 14.03
INSTRUM av-300
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 294.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 0.00 dB
PL1W 32.65452194 W
SFO1 75.4760505 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 120.00 usec
PL2 -3.00 dB
PL12 17.76 dB
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

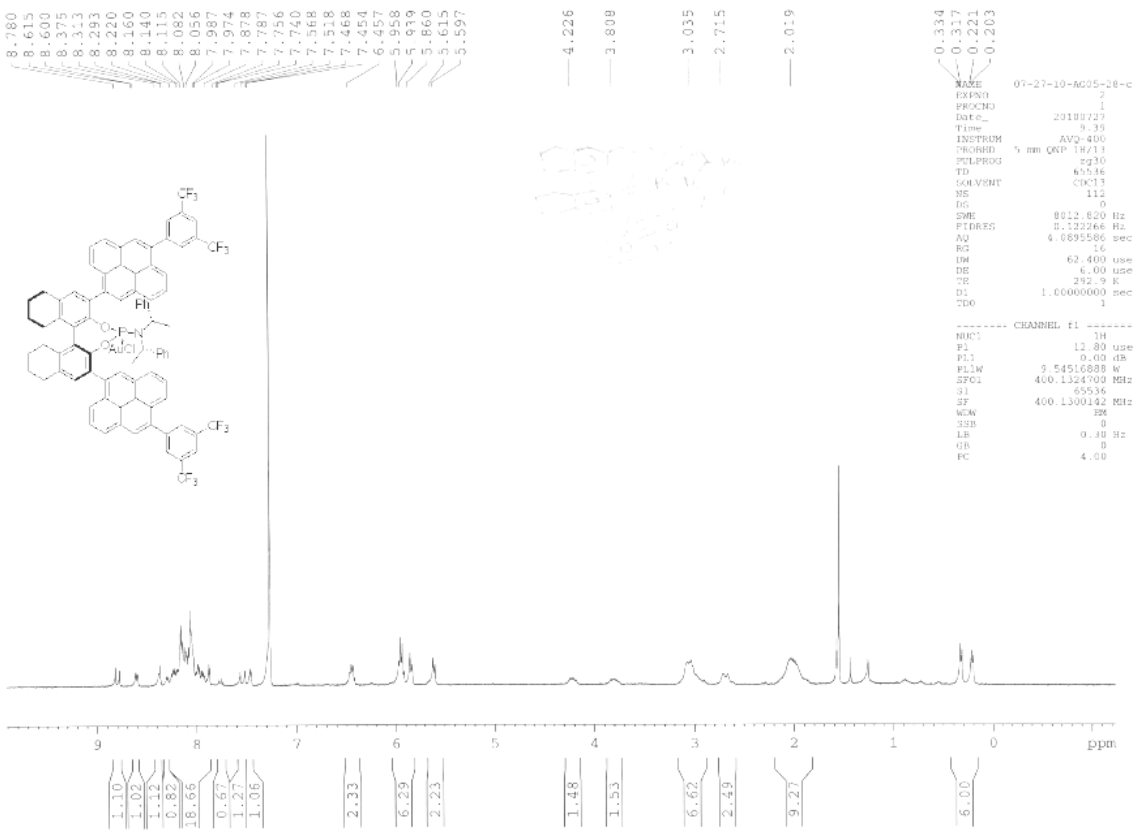

8.032
8.004
7.526
7.233
3.382
3.367
3.352
3.242
3.228
3.216
3.204
3.084
3.069
3.054
2.253
2.239
2.224
2.208
2.134
2.118
2.104
2.090
0.551
F3C
CF3
TMS
NAME 07-07-10-AG05-p10-
EXPNO 1
PROCNO 1
DU /u
USER GonzalezA
Date_ 20100707
Time 15.00
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 64
DW 62.400 use
DE 6.00 use
TE 292.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 =======
NUC1 1H
P1 12.80 use
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
3.00
0.97
1.00
1.97
3.98
2.01
1.96
2.00
8.78

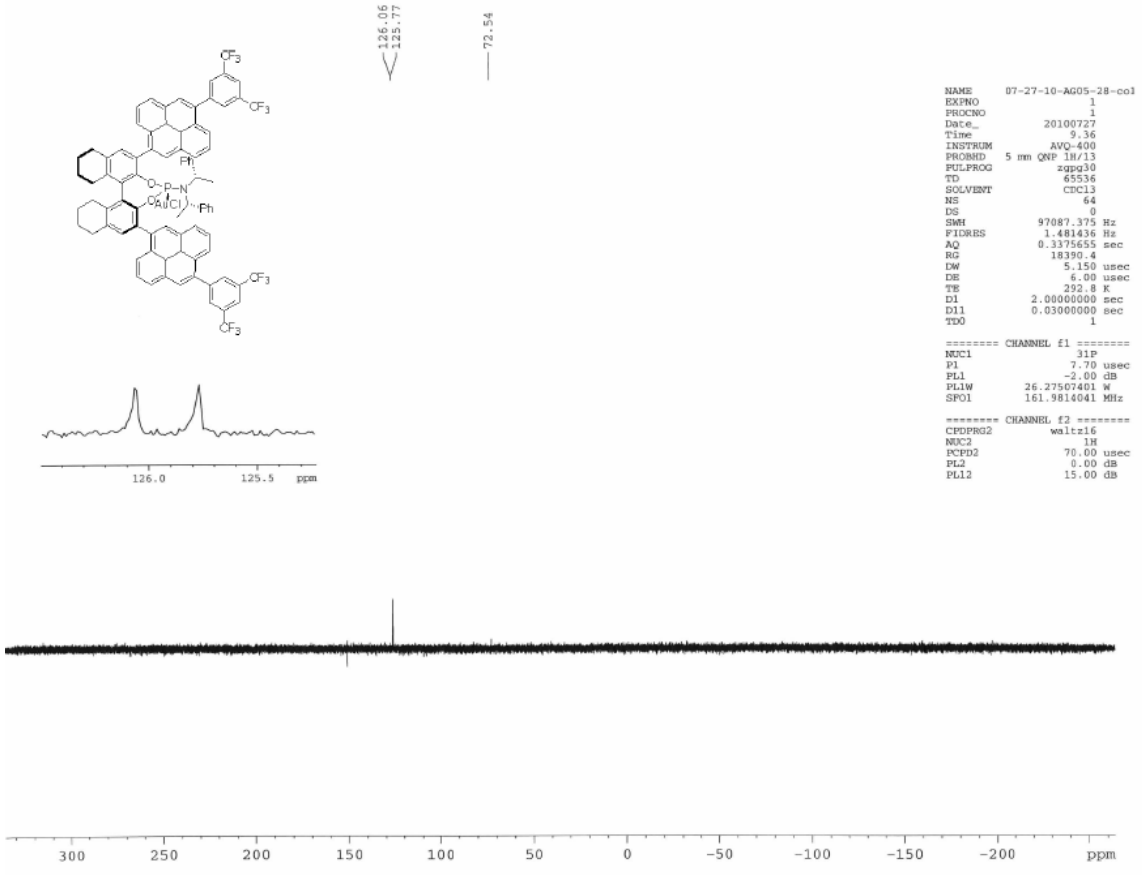

NAME 07-07-10-AG05-p10-col
EXPNO 2
PROCNO 1
DU /u
USER GonzalezA
Date_ 20100707
Time 15.03
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 80
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3632196 sec
RG 16384
DW 20.800 usec
DE 6.00 usec
TE 292.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 -2.00 dB
PL1W 47.77286148 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 17.00 dB
PL2W 9.54516888 W
PL12W 0.30184472 W
PL13W 0.19045115 W
SFO2 400.1316000 MHz
SI 32768
SF 100.6127795 MHz
WDW EM
SSB 0
LB 1.50 Hz
GB 0
PC 1.40
144.44
141.02
135.04
134.05
133.49
133.39
131.62
131.29
131.01
130.76
129.88
129.73
129.64
125.17
124.86
122.15
120.60
77.32
77.00
76.68
32.55
31.64
29.62
23.53
23.22
0.20
F3C
CF3
TMS
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

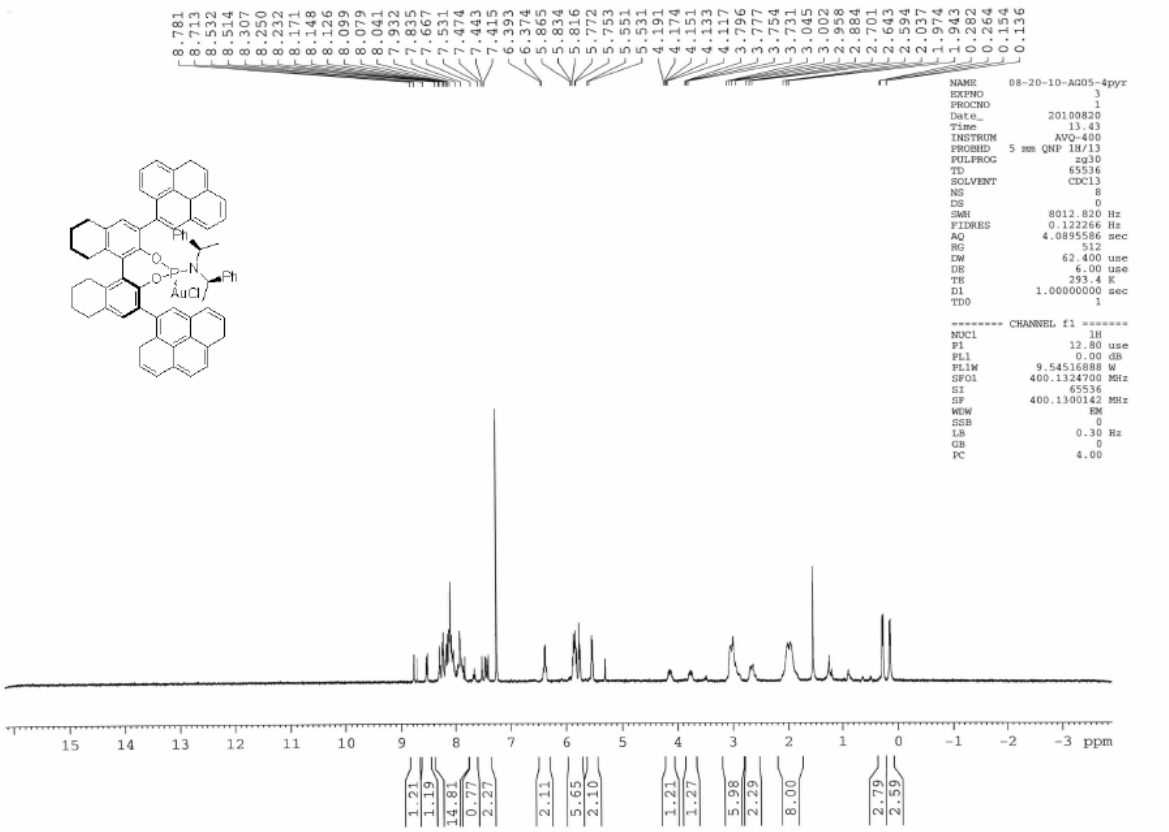

8.672
8.652
8.496
8.334
8.307
8.298
8.270
8.251
8.238
8.192
8.171
8.151
8.125
8.085
8.066
8.047
0.808
F3C
CF3
TMS
Tug
NAME 07-08-10-AG05-12A-
EXPNO 1
PROCNO 1
DU /u
USER GonzalezA
Date_ 20100708
Time 13.09
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 57
DW 62.400 use
DE 6.00 use
TE 292.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 =======
NUC1 1H
P1 12.80 use
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 ppm
1.00
1.03
10.56
9.39

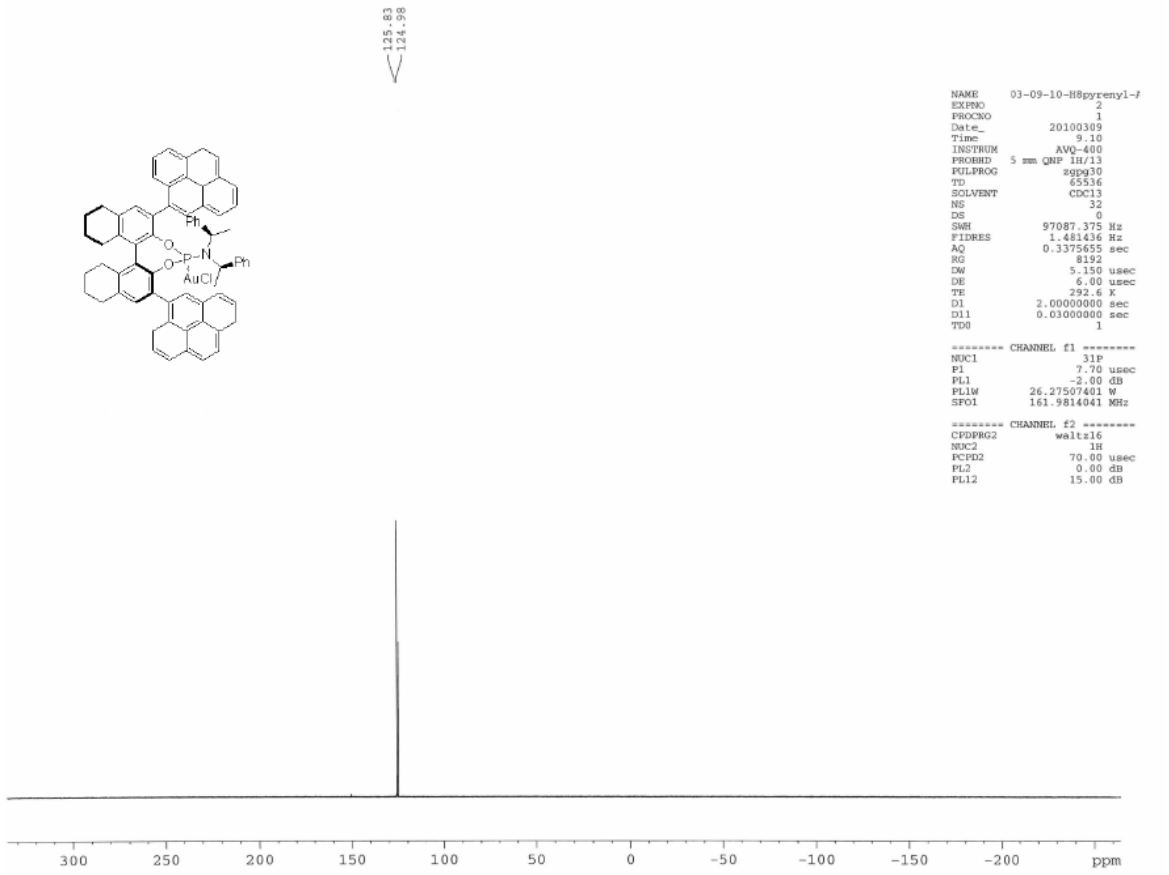

8.811
8.535
8.512
8.509
8.287
8.262
8.166
8.157
8.151
8.145
8.136
8.124
8.099
8.053
8.039
8.009
8.002
7.987
7.252
F3C
CF3
I
NAME 07-08-10-AG05-13-c
EXPNO 1
PROCNO 1
Date_ 20100708
Time 15.28
INSTRUM av-300
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 0
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 645.1
DW 81.000 use
DE 6.00 use
TE 293.8 K
D1 0.20000000 sec
TD0 1
======== CHANNEL f1 =======
NUC1 1H
P1 11.00 use
PL1 -3.00 dB
PL1W 25.05936241 W
SFO1 300.1318533 MHz
SI 32768
SF 300.1300089 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3 ppm
1.00 1.01 1.05 4.11 2.17 1.90

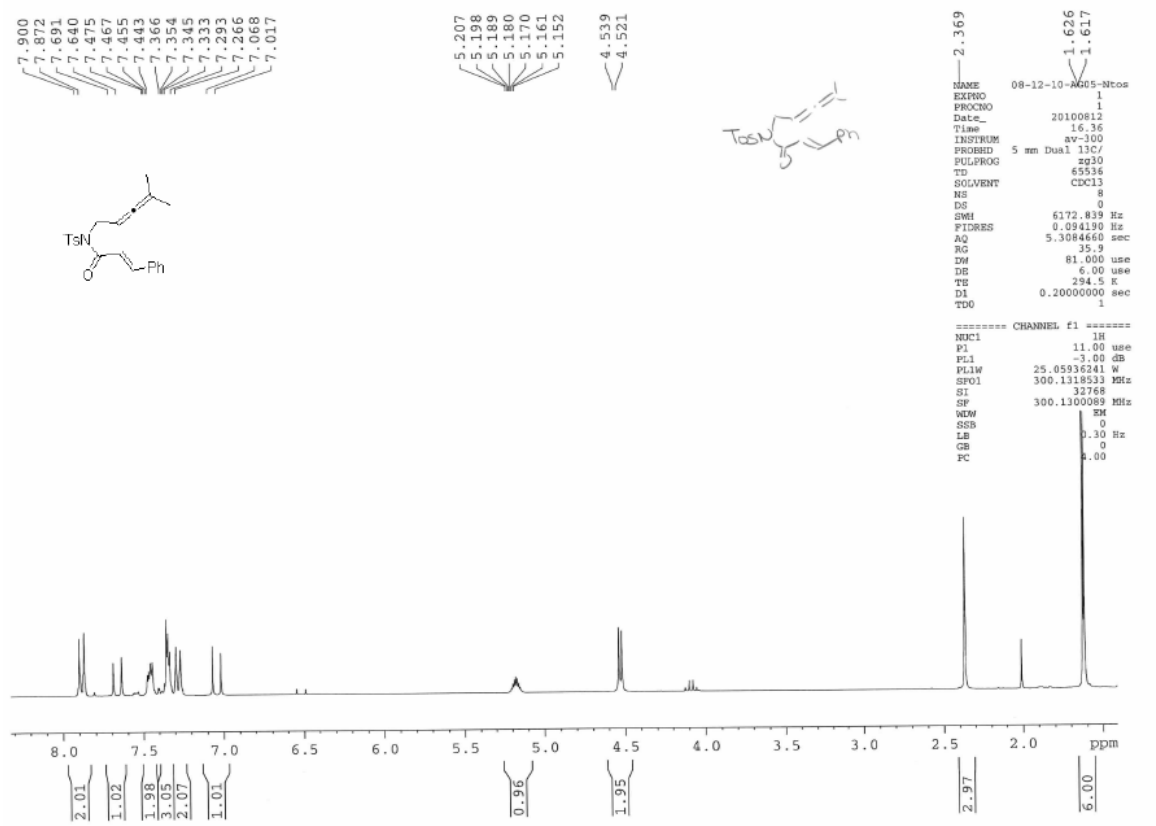

8.200
8.173
8.164
8.159
8.118
8.110
8.099
8.089
8.082
8.055
8.039
8.027
8.019
8.010
7.985
7.966
7.947
7.924
7.905
7.885
7.346
7.335
7.325
5.002
4.954
4.896
4.887
2.915
2.674
2.548
1.940
1.888
CF3
OH
OH
CF3
CF3
NAME 07-12-10-AG05-14-c
EXPNO 1
PROCNO 1
Date_ 20100712
Time 15.03
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 1149.4
DW 62.400 use
DE 6.00 use
TE 292.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 =======
NUC1 1H
P1 12.80 use
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 ppm
2.51 8.49 9.15 0.54 0.65 1.94 1.09 1.15 4.00 4.43 8.14

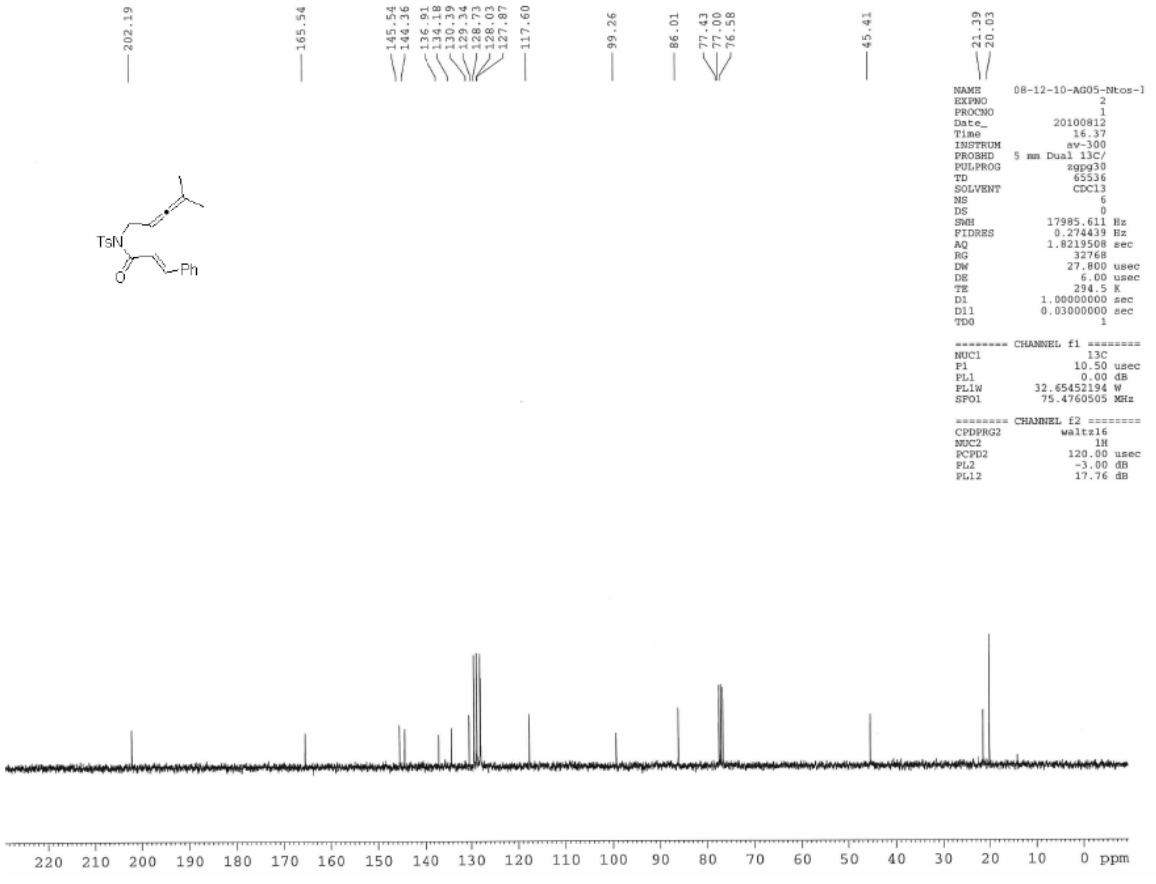


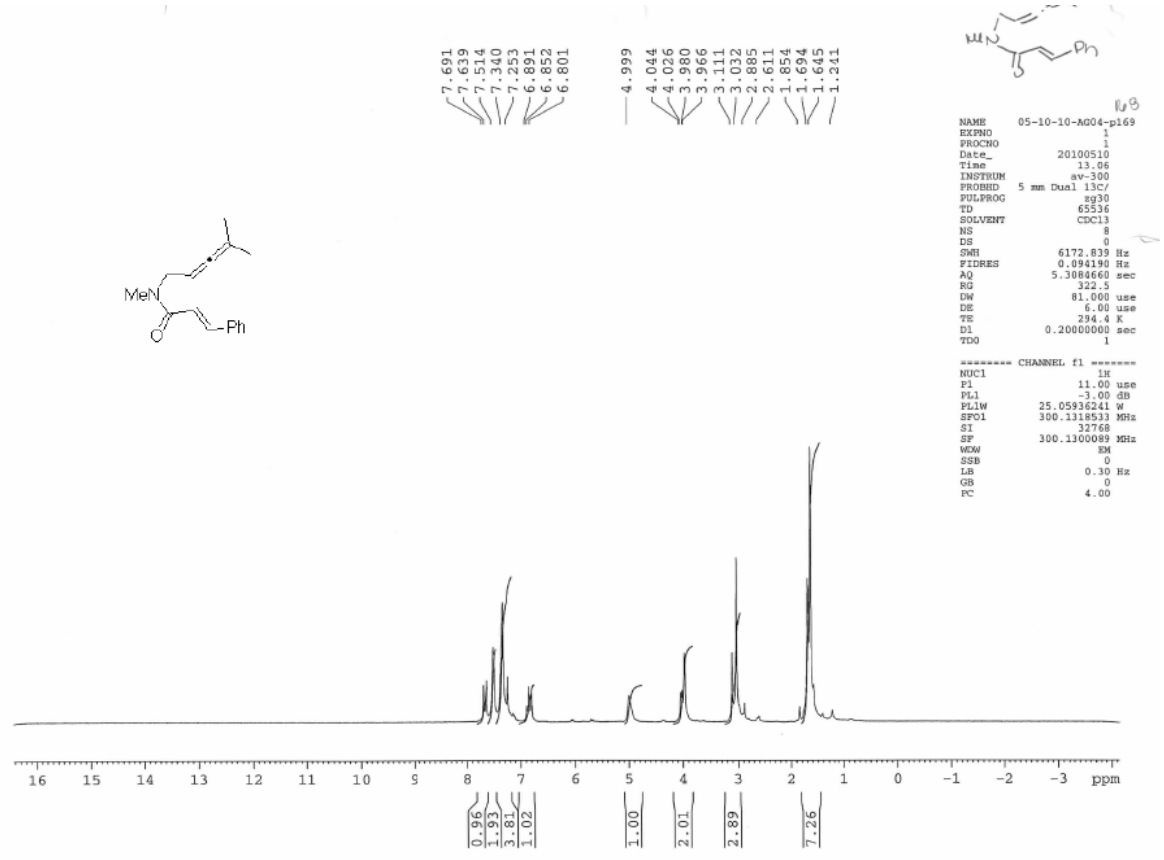


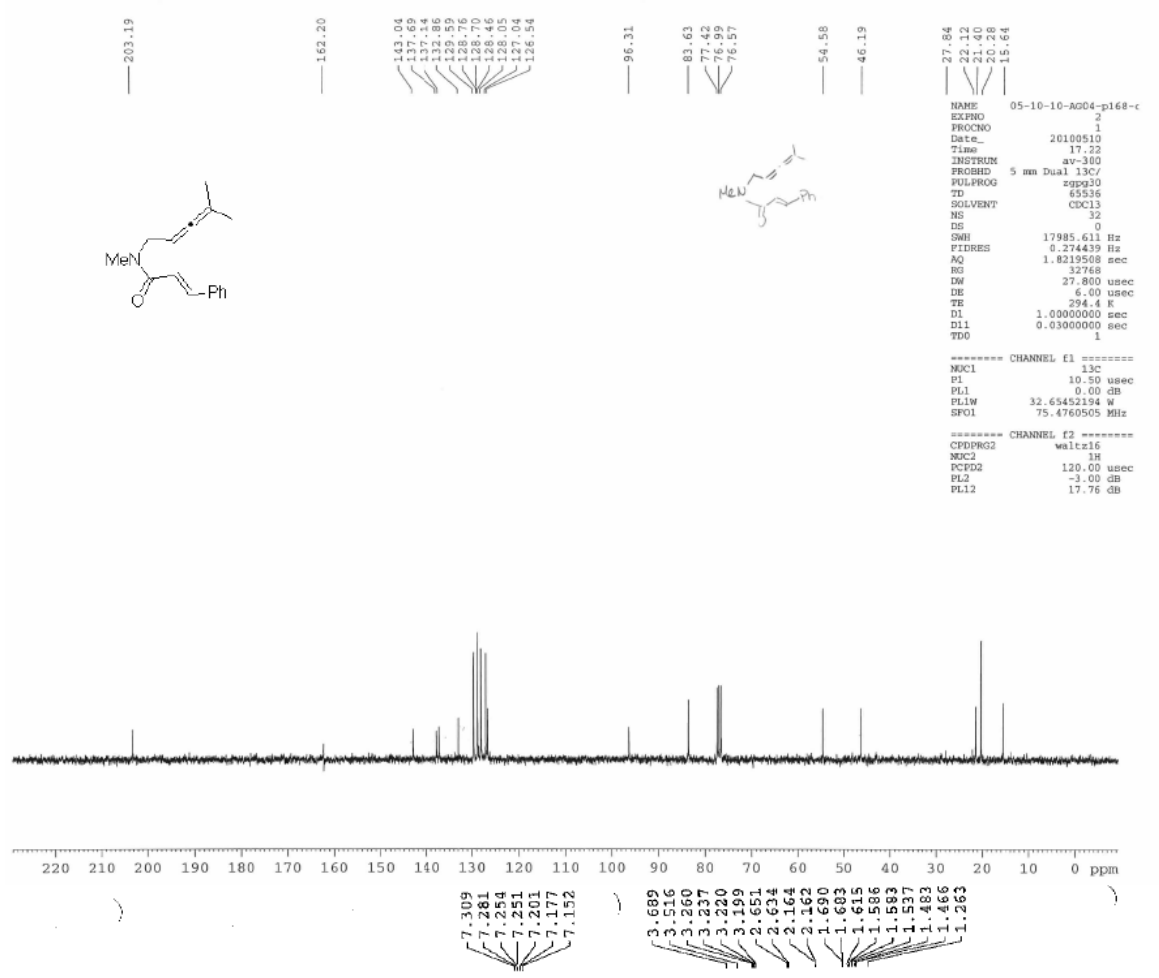

8.781
8.713
8.532
8.514
8.307
8.250
8.232
8.171
8.148
8.126
8.099
8.079
8.041
7.932
7.835
7.667
7.531
7.474
7.443
7.415
6.393
6.374
5.865
5.834
5.816
5.772
5.753
5.551
5.531
4.191
4.174
4.151
4.133
4.117
3.796
3.777
3.754
3.731
3.045
3.002
2.958
2.884
2.701
2.643
2.594
2.037
1.974
1.943
0.282
0.264
0.154
0.136
NAME 08-20-10-AG05-4pyr
EXPNO 3
PROCNO 1
Date_ 20100820
Time 13.43
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 512
DW 62.400 use
DE 6.00 use
TE 293.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 =======
NUC1 1H
P1 12.80 use
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
Ph
O
P
N
Au
Cl
Ph
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 ppm
1.21
1.19
14.81
0.77
2.27
2.11
5.65
2.10
1.21
1.27
5.98
2.29
8.00
2.79
2.59

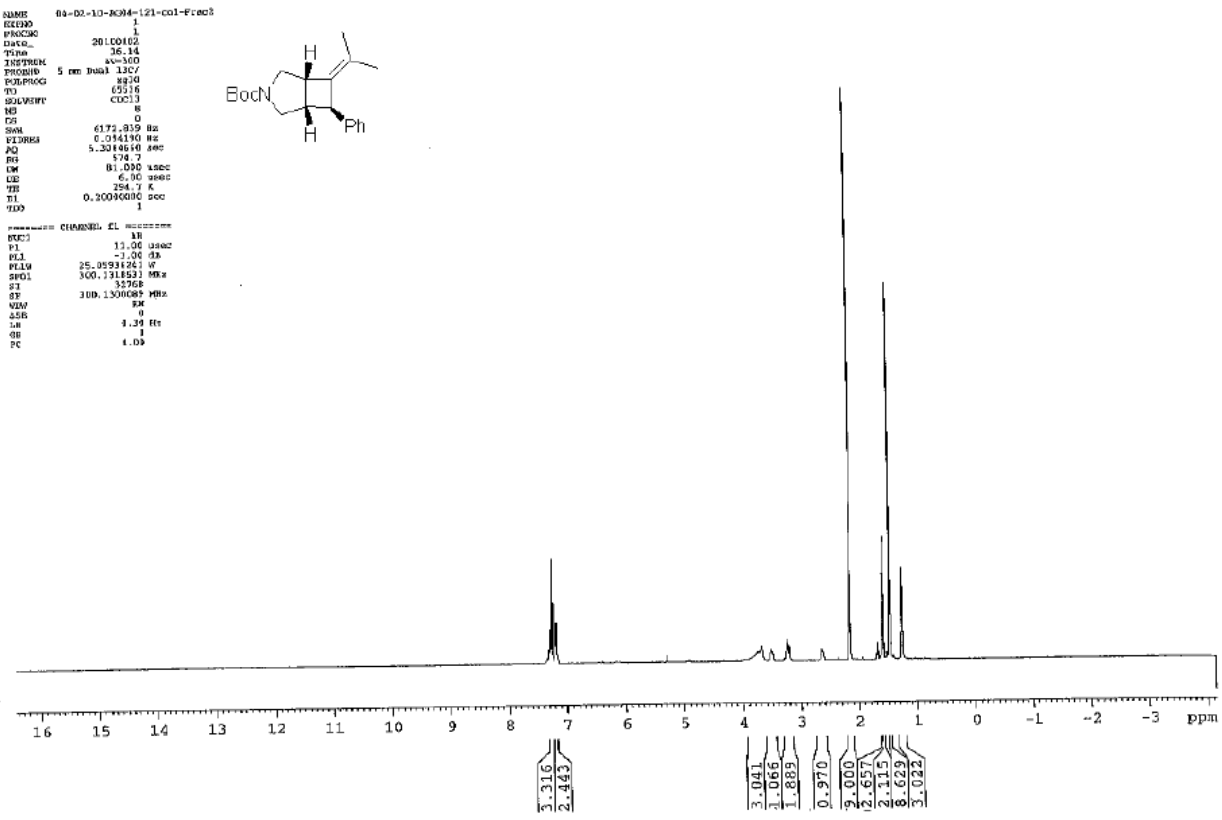

125.83
124.98
NAME 03-09-10-H8pyrenyl-A
EXPNO 2
PROCNO 1
Date_ 20100309
Time 9.10
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 97087.375 Hz
FIDRES 1.481436 Hz
AQ 0.3375655 sec
RG 8192
DW 5.150 usec
DE 6.00 usec
TE 292.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 31P
P1 7.70 usec
PL1 -2.00 dB
PL1W 26.27507401 W
SFO1 161.9814041 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 0.00 dB
PL12 15.00 dB
Ph
O
P
N
Au
Cl
Ph
300 250 200 150 100 50 0 -50 -100 -150 -200 ppm

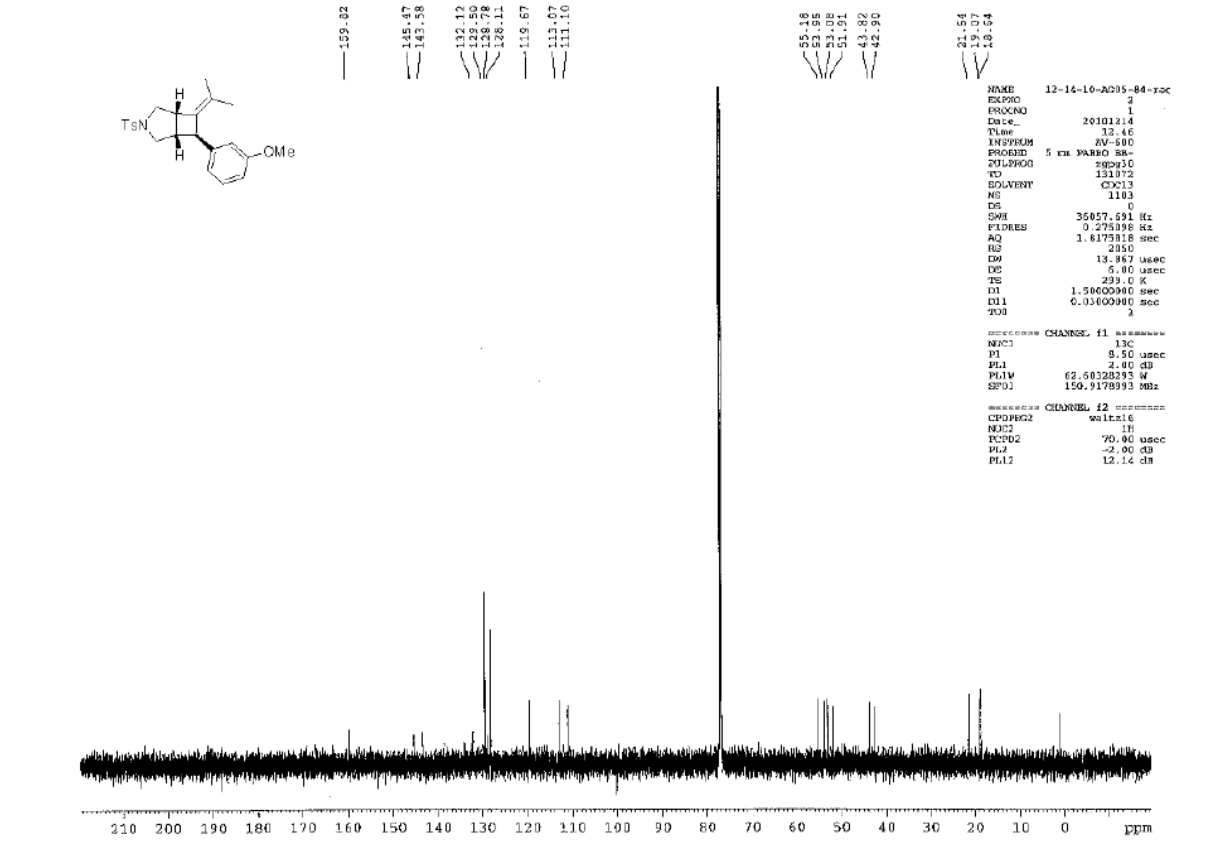

7.900
7.872
7.691
7.640
7.475
7.467
7.455
7.443
7.366
7.354
7.345
7.333
7.293
7.266
7.068
7.017
5.207
5.198
5.189
5.180
5.170
5.161
5.152
4.539
4.521
2.369
1.626
1.617
TsN
Ph
O
NAME 08-12-10-AG05-Ntos
EXPNO 1
PROCNO 1
Date_ 20100812
Time 16.36
INSTRUM av-300
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 35.9
DW 81.000 use
DE 6.00 use
TE 294.5 K
D1 0.20000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.00 use
PL1 -3.00 dB
PL1W 25.05936241 W
SFO1 300.1318533 MHz
SI 32768
SF 300.1300089 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
ppm
2.01
1.02
1.98
3.05
2.07
1.01
0.96
1.95
2.97
6.00

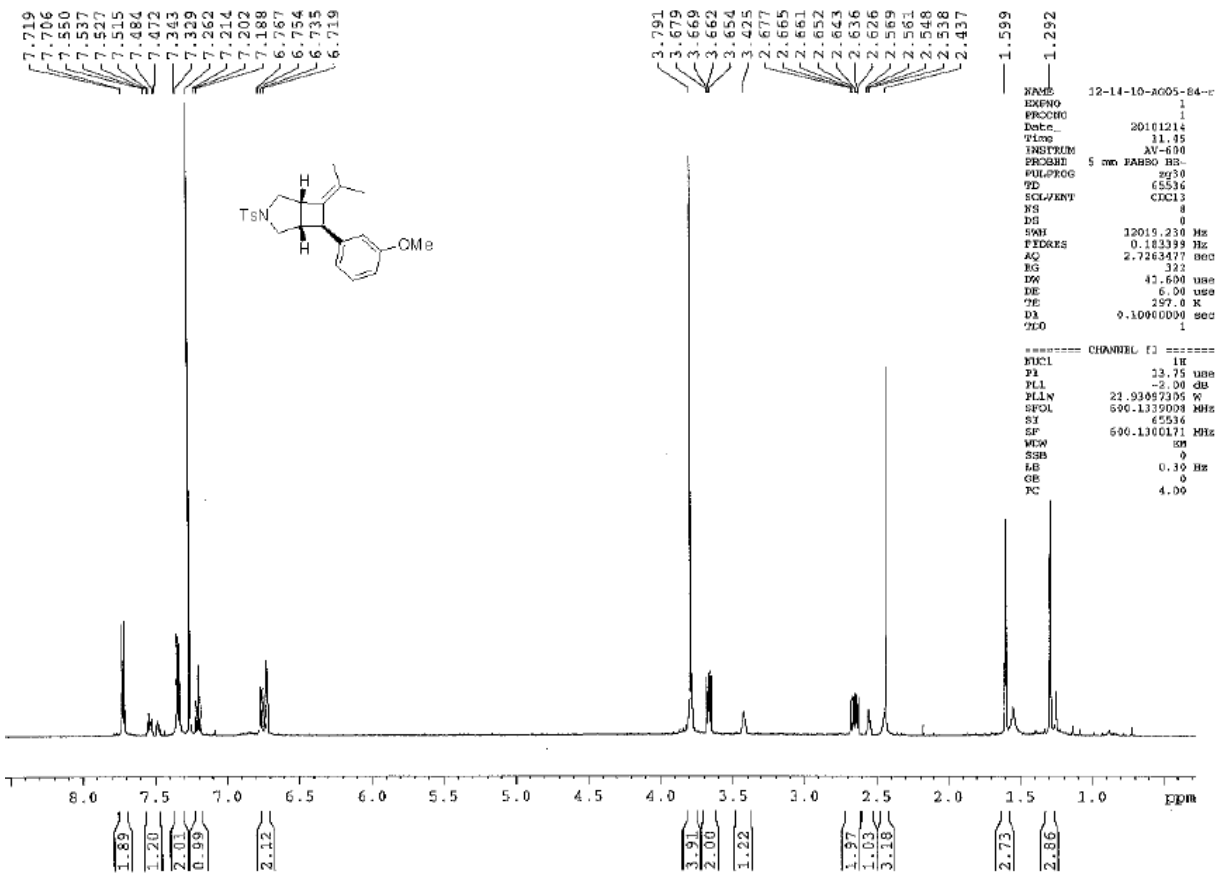

202.19
165.54
145.54
144.36
136.91
134.18
130.39
129.34
128.73
128.03
127.87
117.60
99.26
86.01
77.43
77.00
76.58
45.41
21.39
20.03
TsN
Ph
O
NAME 08-12-10-AG05-Ntos-1
EXPNO 2
PROCNO 1
Date_ 20100812
Time 16.37
INSTRUM av-300
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 294.5 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 0.00 dB
PL1W 32.65452194 W
SFO1 75.4760505 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 120.00 usec
PL2 -3.00 dB
PL12 17.76 dB
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

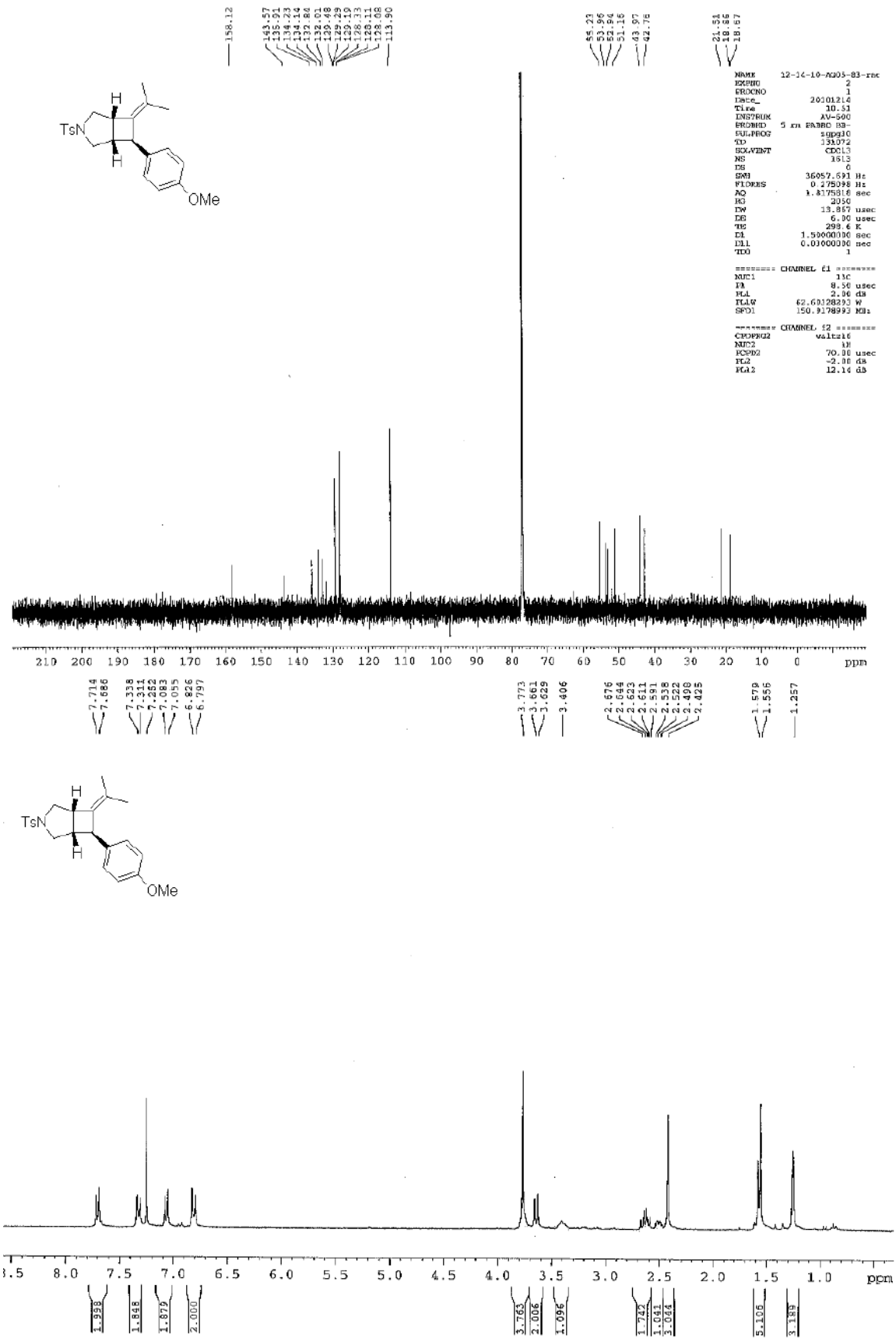

7.691
7.639
7.514
7.340
7.253
6.891
6.852
6.801
4.999
4.044
4.026
3.980
3.966
3.111
3.032
2.885
2.611
1.854
1.694
1.645
1.241
MeN
Ph
NAME 05-10-10-AG04-p169
EXPNO 1
PROCNO 1
Date_ 20100510
Time 13.06
INSTRUM av-300
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 322.5
DW 81.000 use
DE 6.00 use
TE 294.4 K
D1 0.20000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.00 use
PL1 -3.00 dB
PL1W 25.05936241 W
SFO1 300.1318533 MHz
SI 32768
SF 300.1300089 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 ppm
0.96
1.93
3.81
1.02
1.00
2.01
2.89
7.26

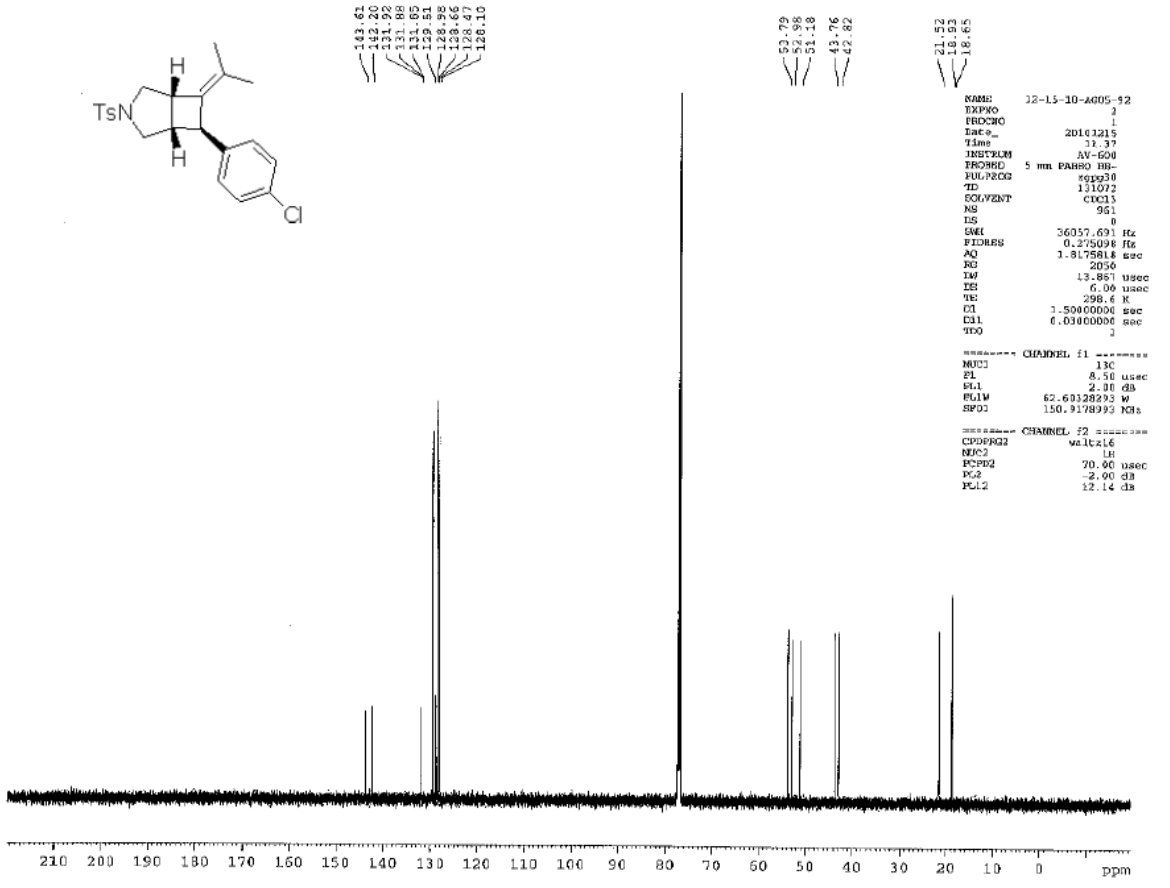

203.19
162.20
143.04
137.69
137.14
132.86
129.59
128.76
128.70
128.46
128.05
127.04
126.54
96.31
83.63
77.42
76.99
76.57
54.58
46.19
27.84
22.12
21.40
20.28
15.64
MeN
Ph
NAME 05-10-10-AG04-p168-c
EXPNO 2
PROCNO 1
Date_ 20100510
Time 17.22
INSTRUM av-300
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 294.4 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 0.00 dB
PL1W 32.65452194 W
SFO1 75.4760505 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 120.00 usec
PL2 -3.00 dB
PL12 17.76 dB
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
7.309
7.281
7.254
7.251
7.201
7.177
7.152
3.689
3.516
3.260
3.237
3.220
3.199
2.651
2.634
2.164
2.162
1.690
1.603
1.615
1.586
1.583
1.537
1.483
1.466
1.263

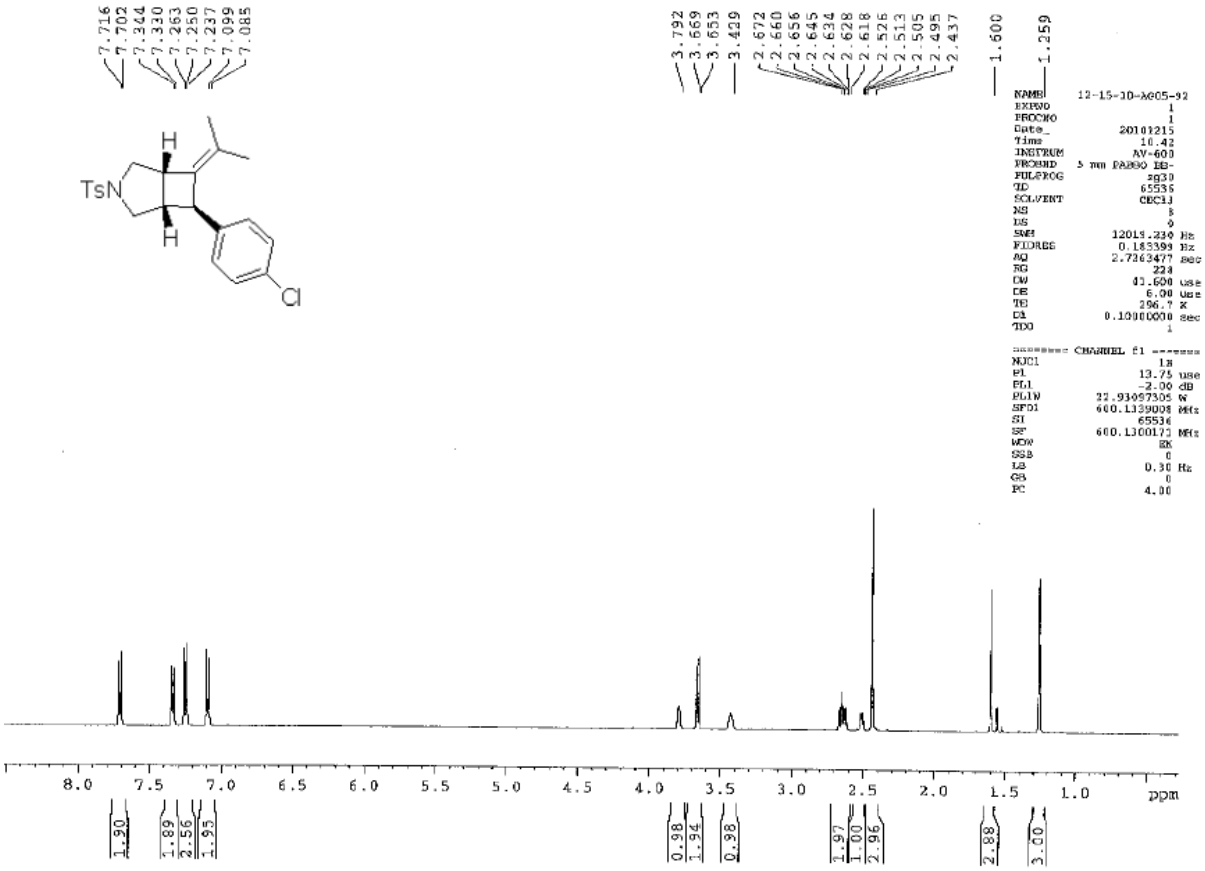

NAME 04-02-10-AG04-121-col-Fract
EXPNO 1
PROCNO 1
Date_ 20100402
Time 16.14
INSTRUM av-300
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3018650 sec
RG 574.7
DW 81.000 usec
DE 6.00 usec
TE 294.7 K
D1 0.20000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -3.00 dB
PL1W 25.05931241 W
SFO1 300.1318521 MHz
SI 32768
SF 300.1300085 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 1
PC 1.00
BocN
H
H
Ph
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 ppm
3.316
2.443
3.041
1.066
1.889
0.970
9.000
2.657
2.115
8.629
3.022

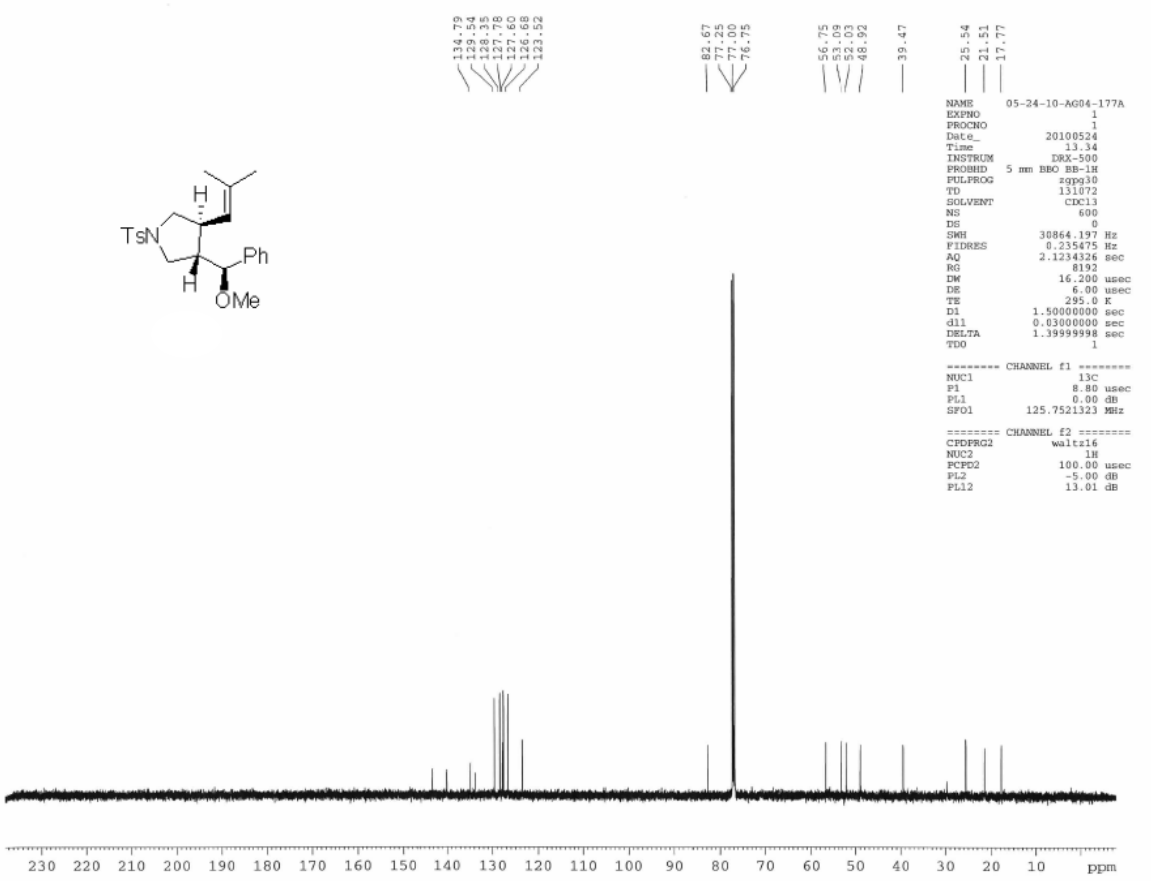

159.82
145.47
143.58
132.12
129.50
128.78
126.11
119.67
113.07
111.10
55.18
53.95
53.08
51.91
43.82
42.90
21.54
19.07
18.64
TsN
OMe
NAME 12-14-10-AG05-84-roc
EXPNO 2
PROCNO 1
Date_ 20101214
Time 12.46
INSTRUM AV-600
PROBHD 5 mm PABBO BB-
PULPROG zgdpg30
TD 131072
SOLVENT CDCl3
NS 1103
DS 0
SWH 36057.691 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2850
DW 13.867 usec
DE 6.00 usec
TE 299.0 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 2.00 dB
PL1W 62.60328293 W
SFO1 150.9178993 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -2.00 dB
PL12 12.14 dB
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

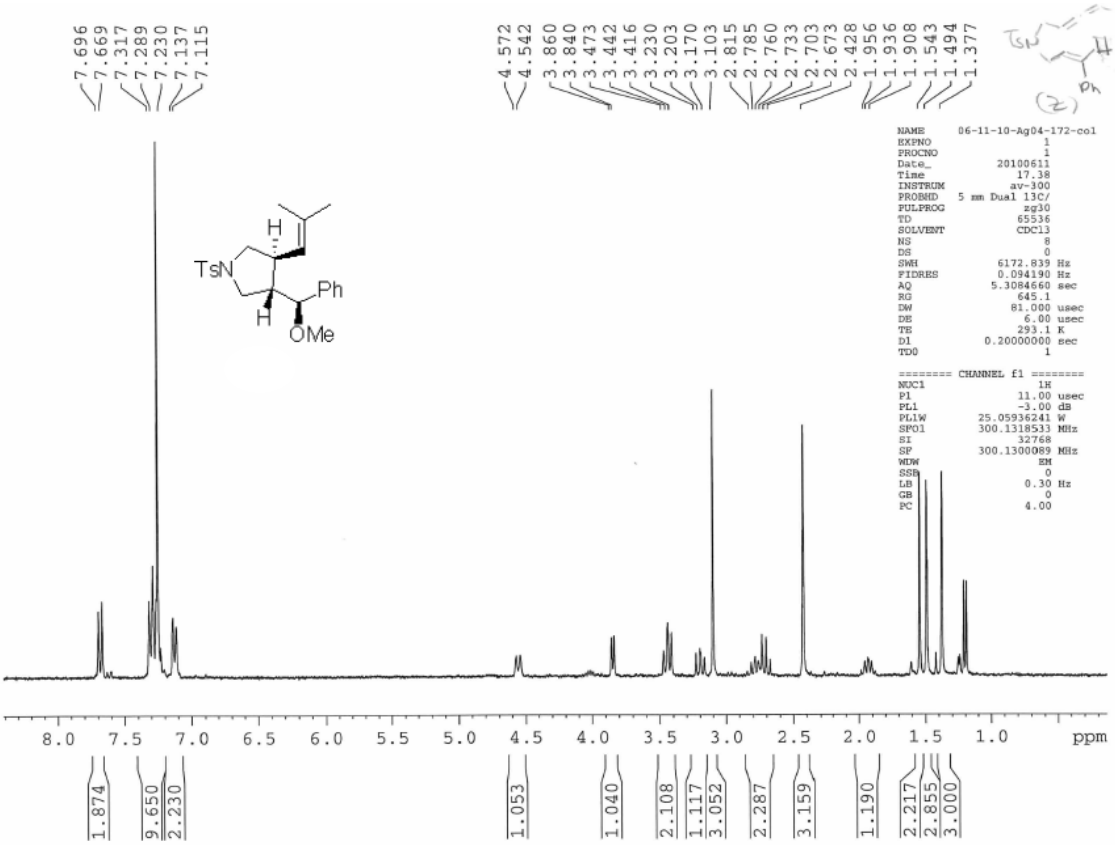

7.719
7.706
7.550
7.537
7.527
7.515
7.484
7.472
7.343
7.329
7.262
7.214
7.202
7.188
6.767
6.754
6.735
6.719
3.791
3.679
3.669
3.662
3.654
3.425
2.677
2.665
2.661
2.652
2.643
2.636
2.626
2.569
2.561
2.548
2.538
2.437
1.599
1.292
TsN
OMe
NAME 12-14-10-AG05-84-r
EXPNO 1
PROCNO 1
Date_ 20101214
Time 11.45
INSTRUM AV-600
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 322
DW 41.600 usec
DE 6.00 usec
TE 297.0 K
D1 0.10000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.75 usec
PL1 -2.00 dB
PL1N 22.93697305 W
SFO1 600.1339008 MHz
SI 65536
SF 600.1300171 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.89
1.20
2.03
0.99
2.12
3.91
2.00
1.22
1.97
1.03
3.18
2.73
2.86

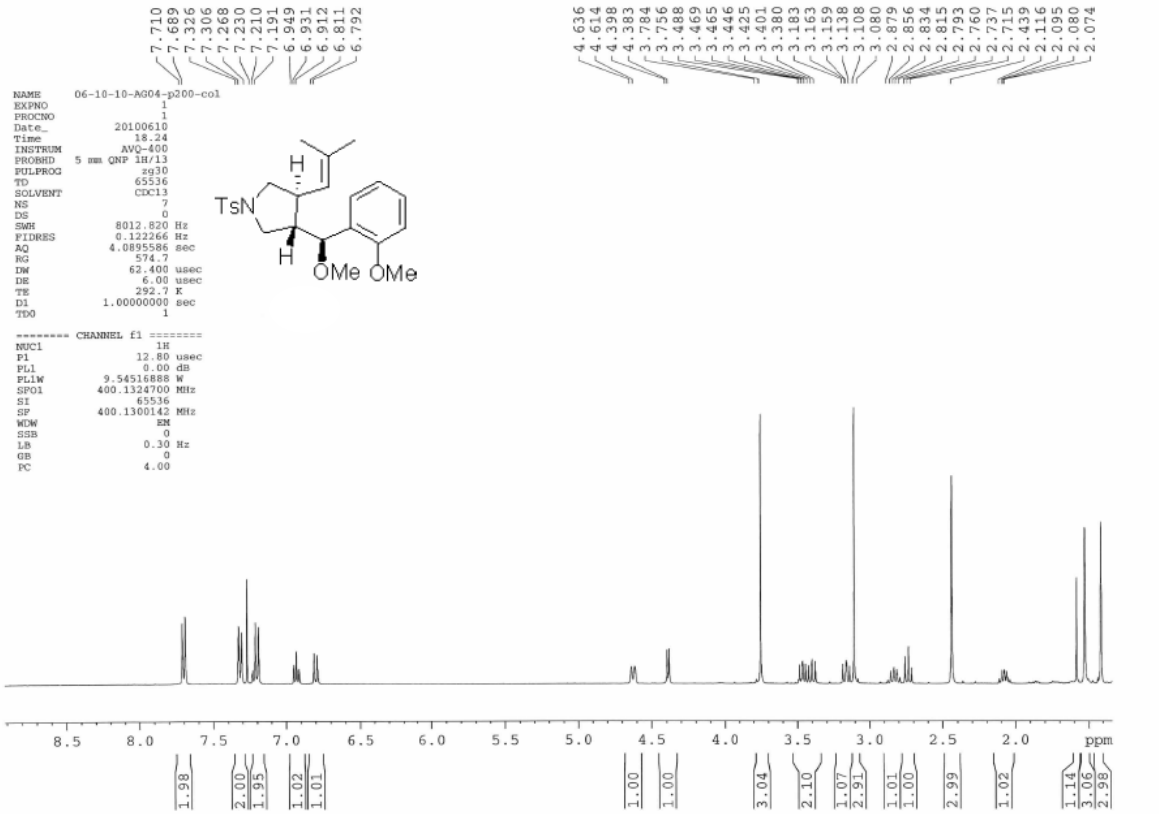

TsN
H
H
OMe
158.12
143.57
135.91
134.23
134.14
132.84
130.01
129.48
129.29
129.19
128.33
128.11
128.08
113.90
55.23
53.66
53.36
51.16
43.97
42.78
21.54
18.86
18.67
NAME 12-14-10-AG05-83-rec
EXPNO 2
PROCNO 1
Date_ 20101214
Time 10.51
INSTRUM AV-500
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 131072
SOLVENT CDCL3
NS 1613
DS 0
SWH 36057.691 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 13.867 usec
DE 6.00 usec
TE 298.6 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 2.00 dB
PL1W 62.60328293 W
SFO1 150.9178993 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -2.00 dB
PL12 12.14 dB
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
7.714
7.686
7.338
7.311
7.282
7.083
7.055
6.826
6.797
3.773
3.661
3.629
3.406
2.676
2.644
2.623
2.611
2.591
2.538
2.522
2.490
2.425
1.578
1.556
1.257
TsN
H
H
OMe
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.938
1.848
1.879
2.000
3.763
2.006
1.096
1.742
1.041
3.084
5.106
3.189

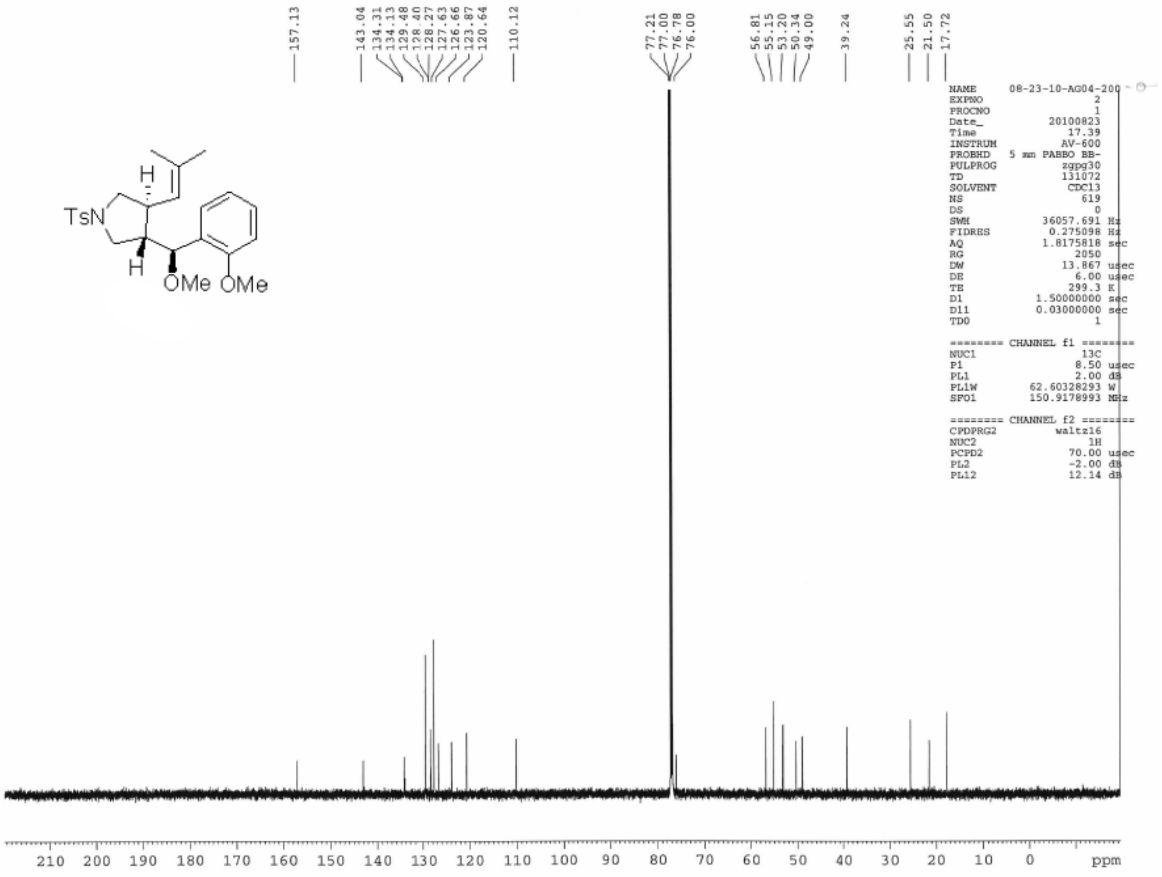

TsN
H
H
Cl
143.61
142.20
131.92
131.88
131.65
129.51
128.98
128.66
128.47
126.10
59.79
52.98
51.18
43.76
42.82
21.52
18.93
18.65
NAME 12-15-10-AG05-92
EXPNO 2
PROCNO 1
Date_ 20101215
Time 11.37
INSTRUM AV-600
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 961
DS 0
SWH 36057.691 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 13.861 usec
DE 6.00 usec
TE 298.6 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 2.00 dB
PL1W 62.60328293 W
SFO1 150.9178993 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -2.90 dB
PL12 12.14 dB
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

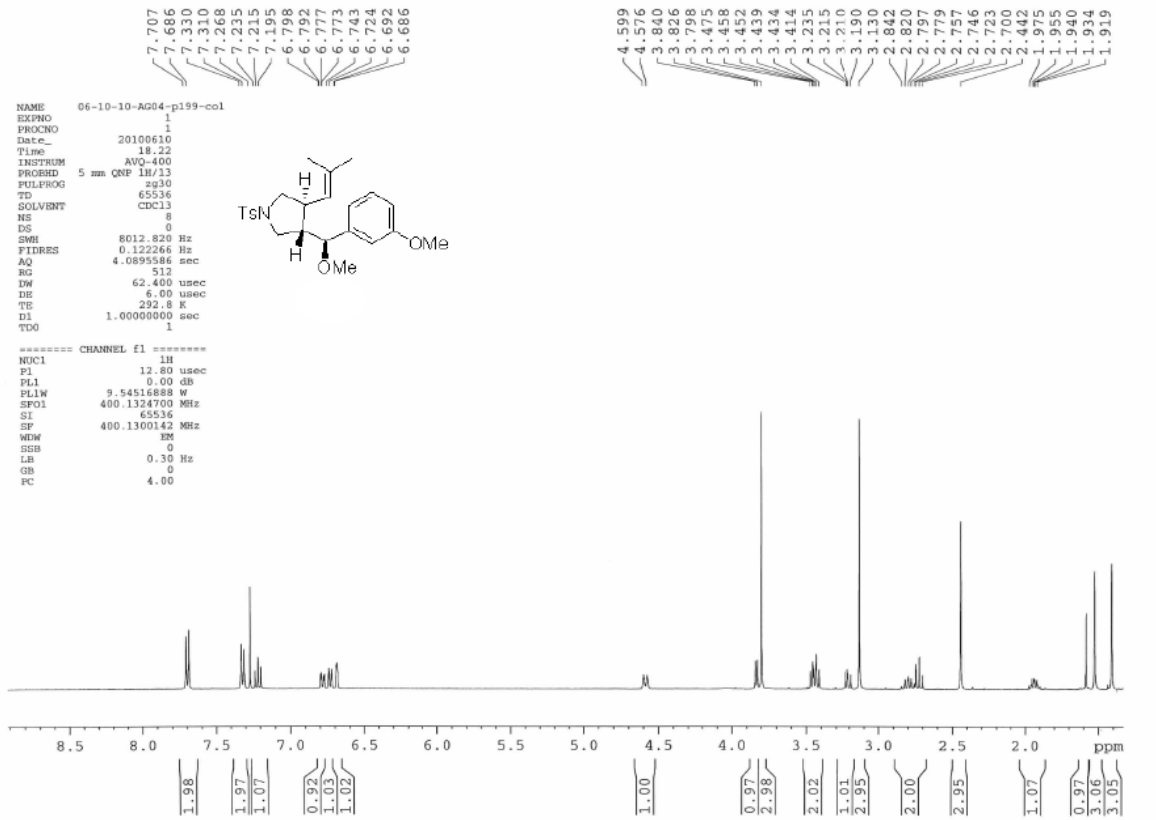

7.716
7.702
7.344
7.330
7.263
7.250
7.237
7.099
7.085
3.792
3.669
3.653
3.439
2.672
2.660
2.656
2.645
2.634
2.628
2.618
2.526
2.513
2.505
2.495
2.437
1.600
1.259
TsN
H
H
Cl
NAME 12-15-10-AG05-92
EXPNO 1
PROCNO 1
Date_ 20101215
Time 10.42
INSTRUM AV-600
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 228
DW 41.600 usec
DE 6.00 usec
TE 296.7 K
D1 0.10000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.75 usec
PL1 -2.00 dB
PL1W 22.93097305 W
SFO1 600.1339008 MHz
SI 65536
SF 600.1300173 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.90
1.89
2.56
1.93
0.98
1.94
0.98
1.97
1.00
2.96
2.88
3.00

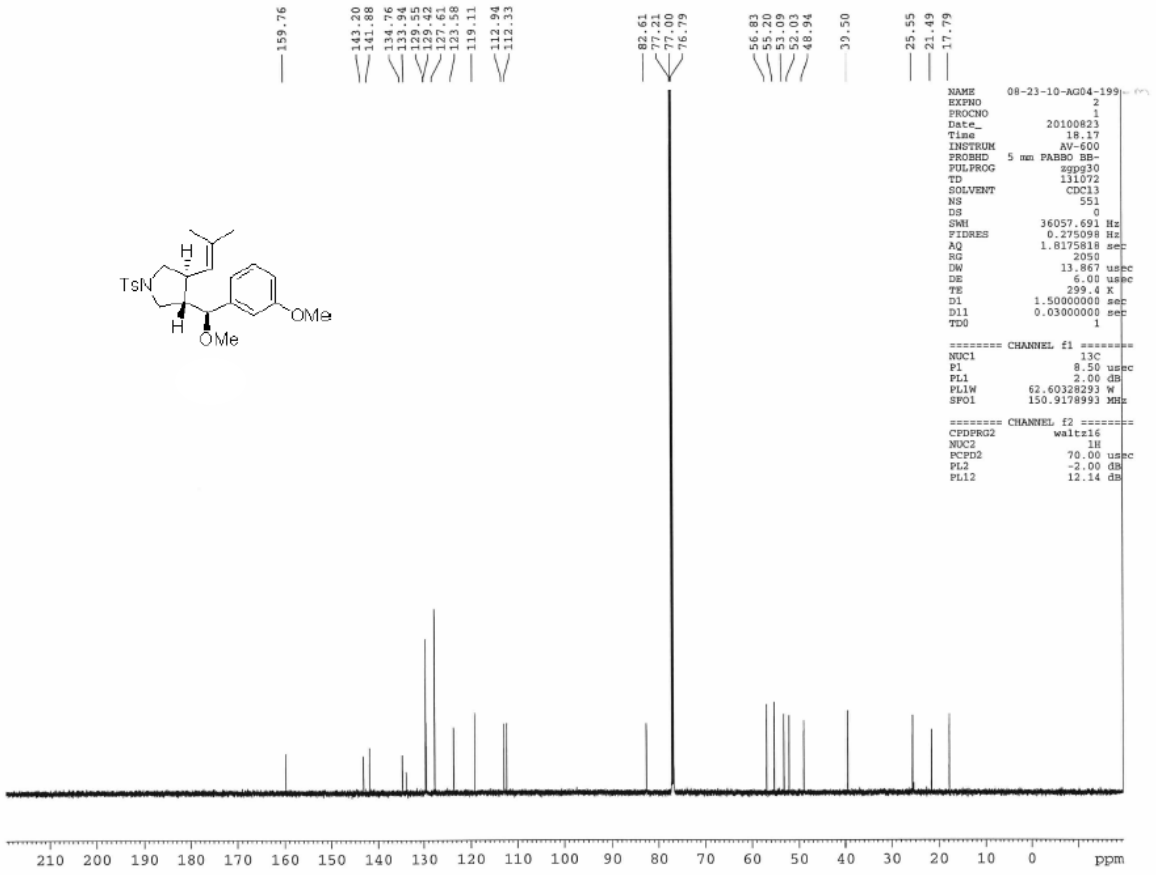

134.79
129.54
128.35
127.78
127.60
126.68
123.52
82.67
77.25
77.00
76.75
56.75
53.09
52.03
48.92
39.47
25.54
21.51
17.77
NAME 05-24-10-AG04-177A
EXPNO 1
PROCNO 1
Date_ 20100524
Time 13.34
INSTRUM DRX-500
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 600
DS 0
SWH 30864.197 Hz
FIDRES 0.235475 Hz
AQ 2.1234326 sec
RG 8192
DW 16.200 usec
DE 6.00 usec
TE 295.0 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.80 usec
PL1 0.00 dB
SFO1 125.7521323 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -5.00 dB
PL12 13.01 dB
TsN
H
Ph
OMe
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

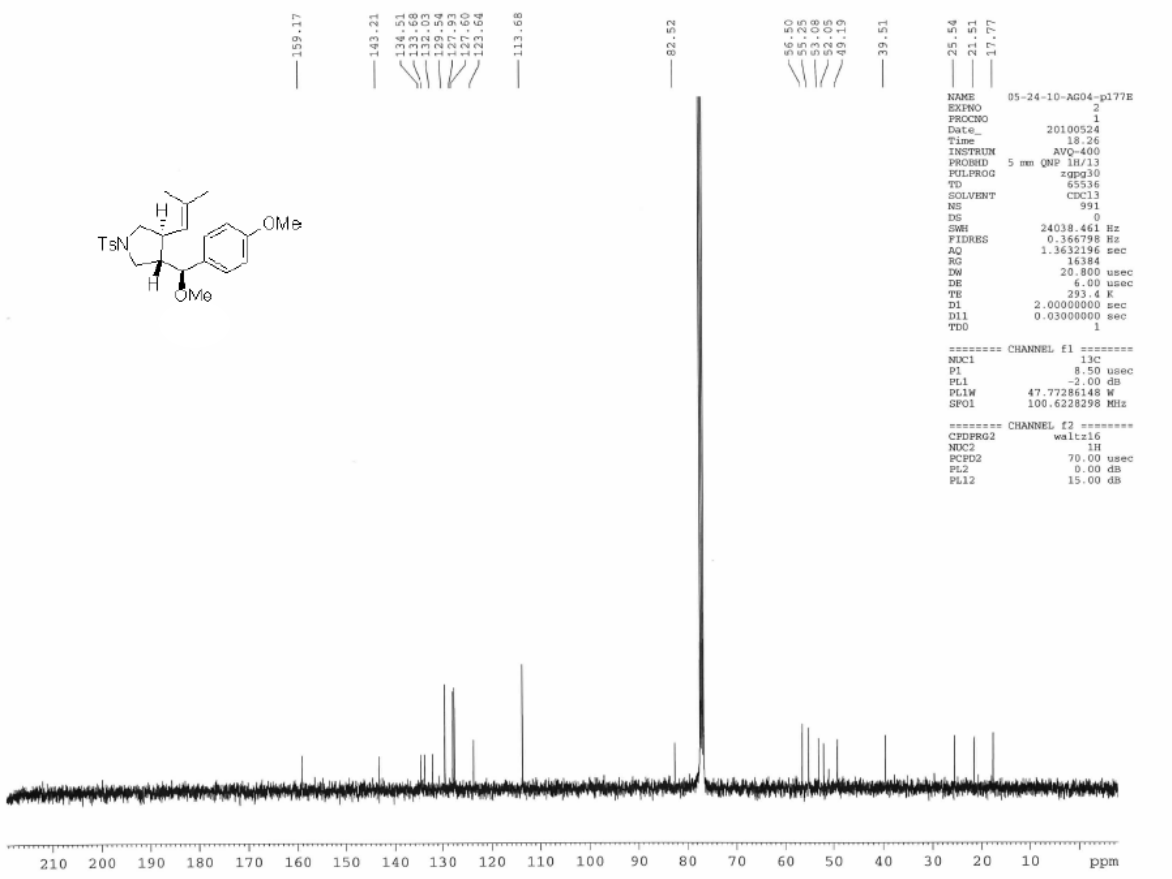

7.696
7.669
7.317
7.289
7.230
7.137
7.115
4.572
4.542
3.860
3.840
3.473
3.442
3.416
3.230
3.203
3.170
3.103
2.815
2.785
2.760
2.733
2.703
2.673
2.428
1.956
1.936
1.908
1.543
1.494
1.377
(Z)
NAME 06-11-10-Ag04-172-col
EXPNO 1
PROCNO 1
Date_ 20100611
Time 17.38
INSTRUM av-300
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 645.1
DW 81.000 usec
DE 6.00 usec
TE 293.1 K
D1 0.20000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -3.00 dB
PL1W 25.05936241 W
SFO1 300.1318533 MHz
SI 32768
SF 300.1300089 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
TsN
H
Ph
OMe
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.874
9.650
2.230
1.053
1.040
2.108
1.117
3.052
2.287
3.159
1.190
2.217
2.855
3.000

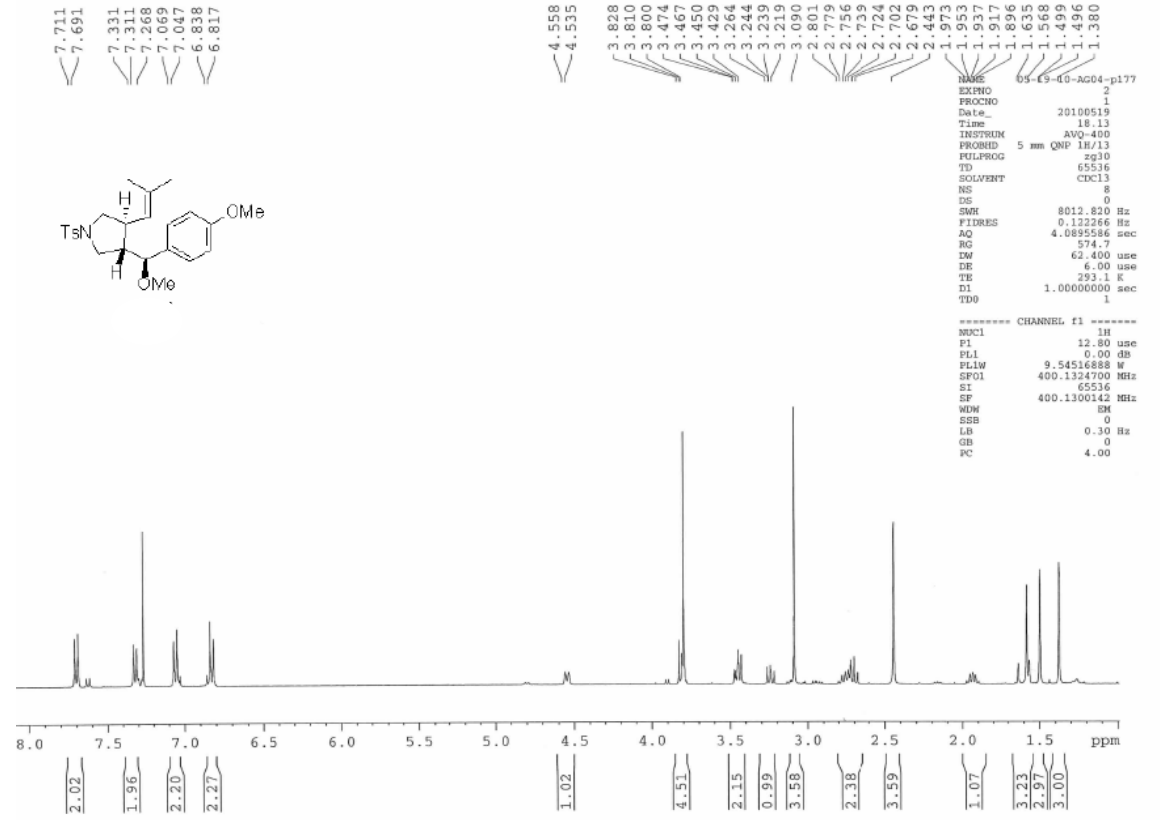

7.710
7.689
7.326
7.306
7.268
7.230
7.210
7.191
6.949
6.931
6.912
6.811
6.792
4.636
4.614
4.398
4.383
4.784
3.756
3.488
3.469
3.465
3.446
3.425
3.401
3.380
3.183
3.163
3.159
3.138
3.108
3.080
2.879
2.856
2.834
2.815
2.793
2.760
2.737
2.715
2.439
2.116
2.095
2.080
2.074
NAME 06-10-10-AG04-p200-col
EXPNO 1
PROCNO 1
Date_ 20100610
Time 18.24
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 7
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 574.7
DW 62.400 usec
DE 6.00 usec
TE 292.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 usec
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
TsN
H
H
OMe OMe
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 ppm
1.98 2.00 1.95 1.02 1.01 1.00 1.00 3.04 2.10 1.07 2.91 1.01 1.00 2.99 1.02 1.14 3.06 2.98

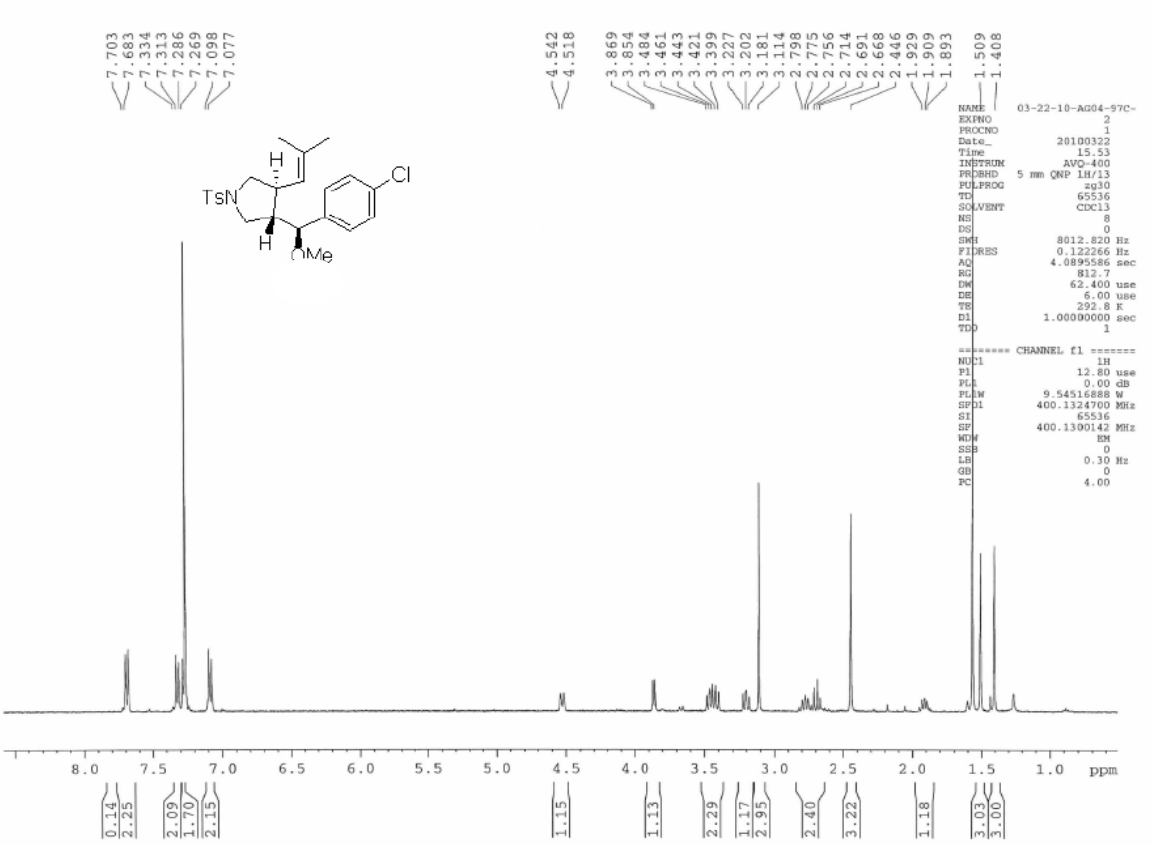

157.13
143.04
134.31
134.13
129.48
128.40
128.27
127.63
126.66
123.87
120.64
110.12
77.21
77.00
76.78
76.00
56.81
55.15
53.20
50.34
49.00
39.24
25.55
21.50
17.72
NAME 08-23-10-AG04-200
EXPNO 2
PROCNO 1
Date_ 20100823
Time 17.39
INSTRUM AV-600
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 619
DS 0
SWH 36057.691 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 13.867 usec
DE 6.00 usec
TE 299.3 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 2.00 dB
PL1W 62.60328293 W
SFO1 150.9178993 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -2.00 dB
PL12 12.14 dB
TsN
H
H
OMe OMe
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

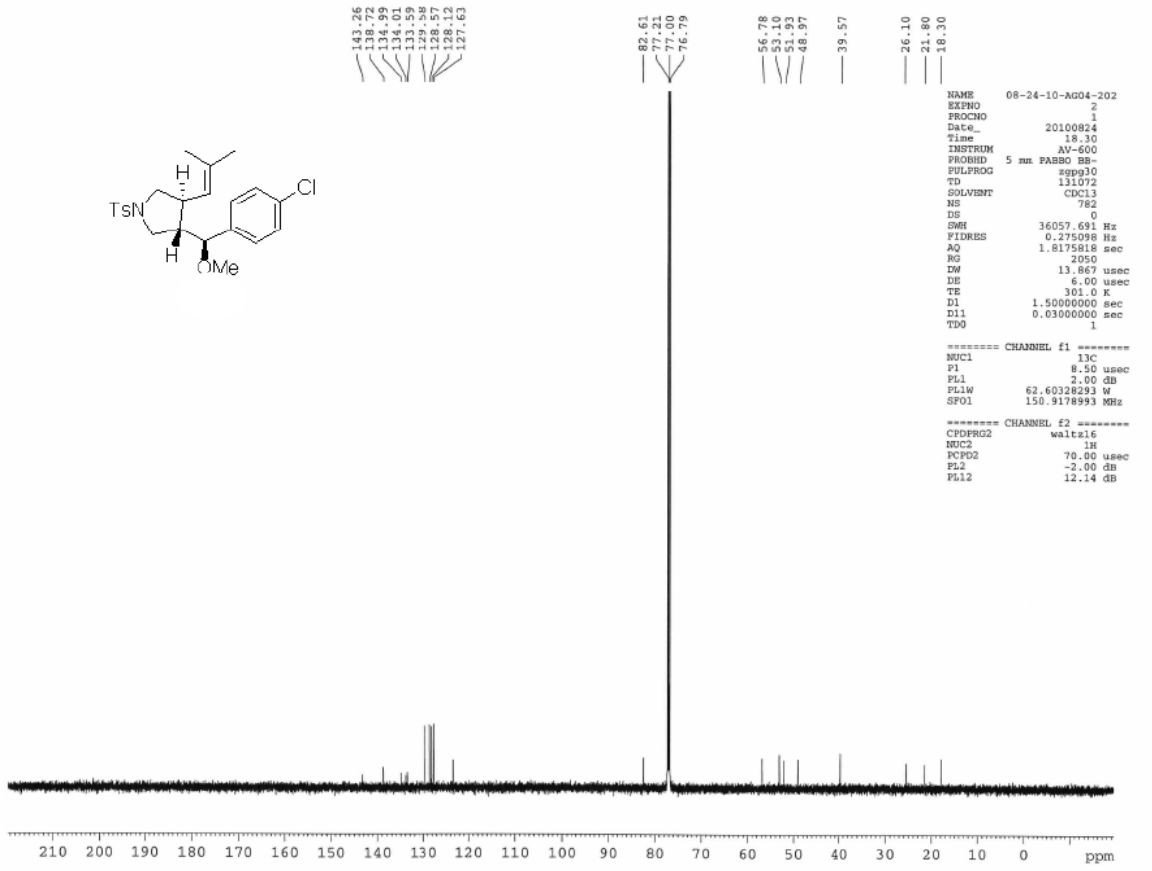

7.707
7.686
7.330
7.310
7.268
7.235
7.215
7.195
6.798
6.792
6.777
6.773
6.743
6.724
6.692
6.686
4.599
4.576
3.840
3.826
3.798
3.475
3.458
3.452
3.439
3.434
3.414
3.235
3.215
3.210
3.190
3.130
2.842
2.820
2.797
2.779
2.757
2.746
2.723
2.700
2.442
1.975
1.955
1.940
1.934
1.919
NAME 06-10-10-AG04-p199-col
EXPNO 1
PROCNO 1
Date_ 20100610
Time 18.22
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 512
DW 62.400 usec
DE 6.00 usec
TE 292.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 usec
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
TsN
H
H
OMe
OMe
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
ppm
1.98
1.97
1.07
0.92
1.03
1.02
1.00
0.97
2.98
2.02
1.01
2.95
2.00
2.95
1.07
0.97
3.06
3.05

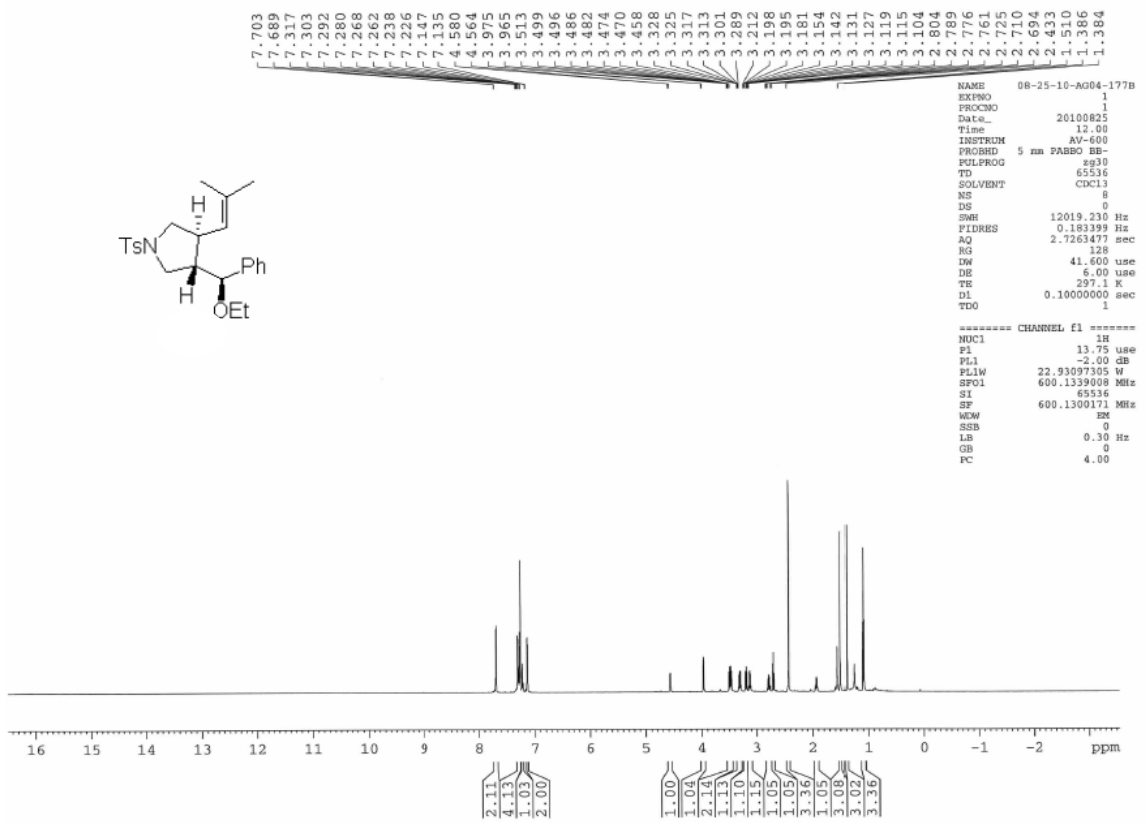

159.76
143.20
141.88
134.76
133.94
129.55
129.42
127.61
123.58
119.11
112.94
112.33
82.61
77.21
77.00
76.79
56.83
55.20
53.09
52.03
48.94
39.50
25.55
21.49
17.79
NAME 08-23-10-AG04-199
EXPNO 2
PROCNO 1
Date_ 20100823
Time 18.17
INSTRUM AV-600
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 551
DS 0
SWH 36057.691 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 13.867 usec
DE 6.00 usec
TE 299.4 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 2.00 dB
PL1W 62.60328293 W
SFO1 150.9178993 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -2.00 dB
PL12 12.14 dB
TsN
H
H
OMe
OMe
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

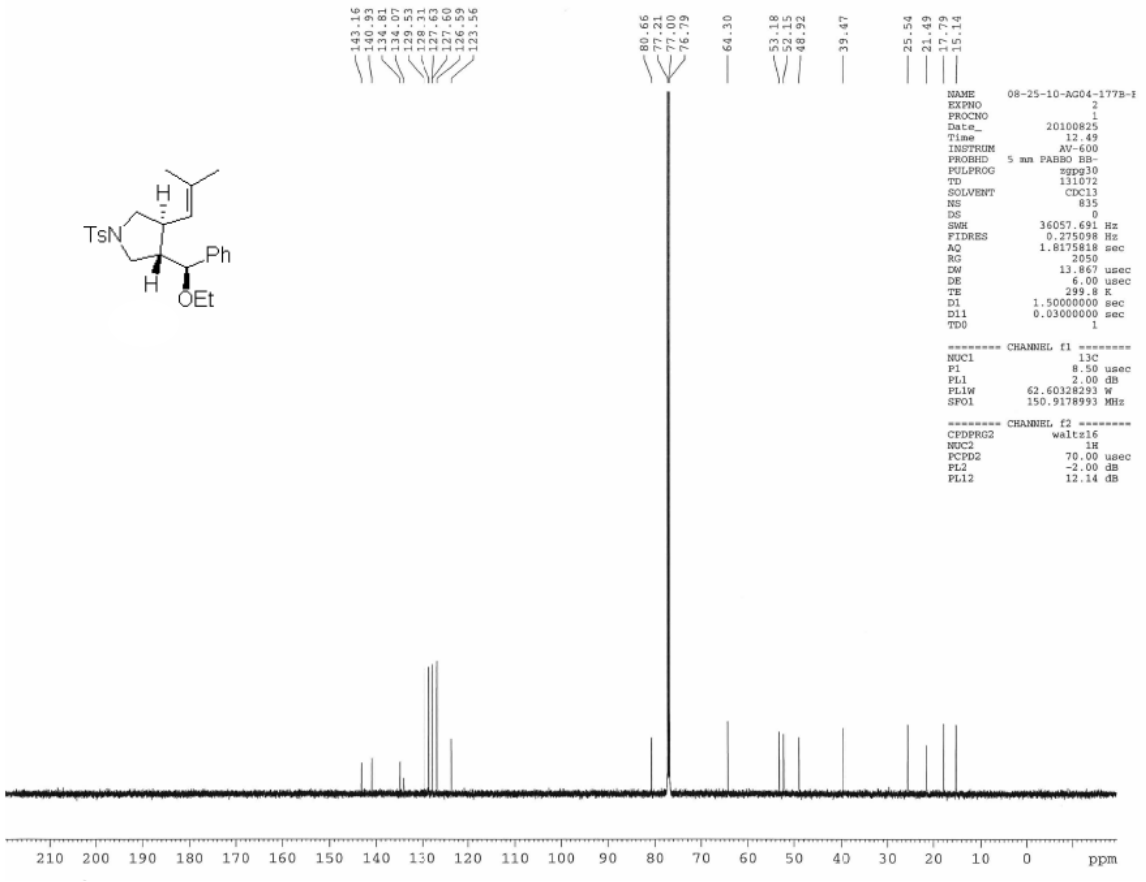

159.17
143.21
134.51
133.68
132.03
129.54
127.93
127.60
123.64
113.68
82.52
56.50
55.25
53.08
52.05
49.19
39.51
25.54
21.51
17.77
TsN
OMe
OMe
H
H
NAME 05-24-10-AG04-p177E
EXPNO 2
PROCNO 1
Date_ 20100524
Time 18.26
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 991
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3632196 sec
RG 16384
DW 20.800 usec
DE 6.00 usec
TE 293.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 -2.00 dB
PL1W 47.77286148 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 0.00 dB
PL12 15.00 dB
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

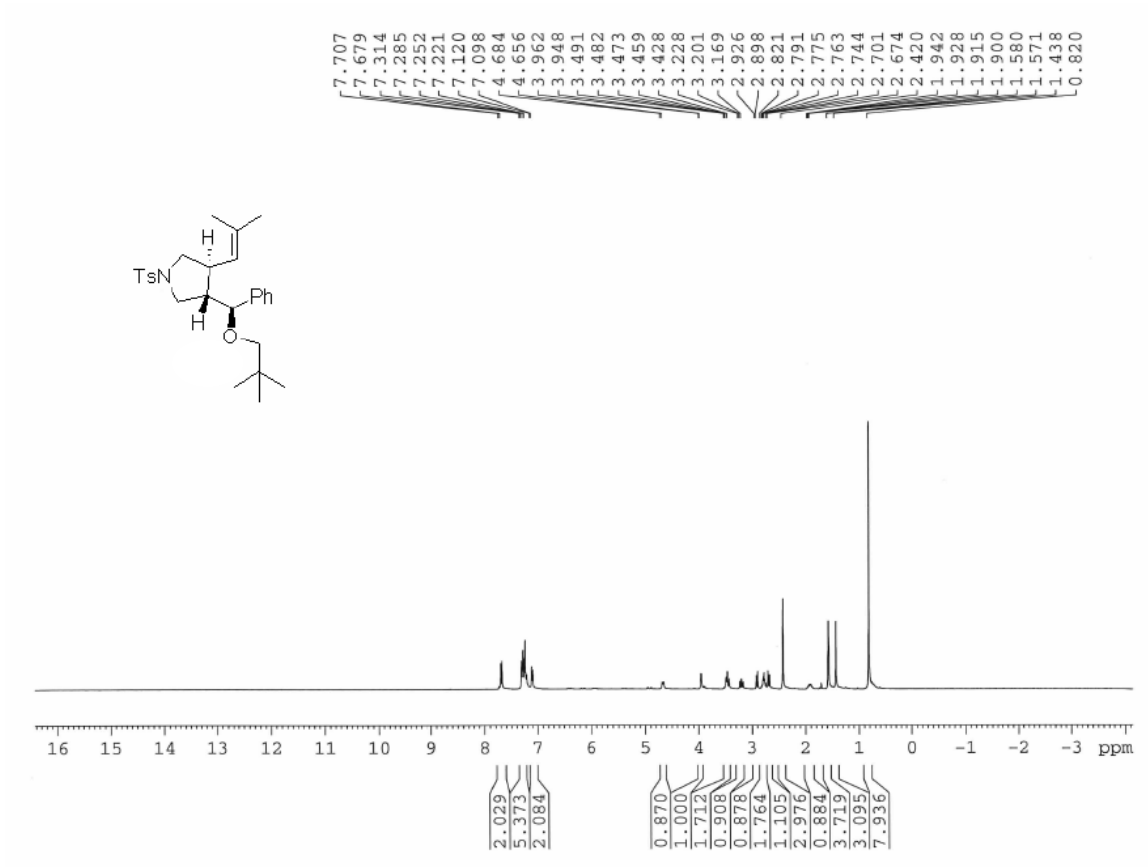

7.711
7.691
7.331
7.311
7.268
7.069
7.047
6.838
6.817
4.558
4.535
3.828
3.810
3.800
3.474
3.467
3.450
3.429
3.264
3.244
3.239
3.219
3.090
2.801
2.779
2.756
2.739
2.724
2.702
2.679
2.443
1.973
1.953
1.937
1.917
1.896
1.635
1.568
1.499
1.496
1.380
TsN
OMe
OMe
H
H
NAME 05-19-10-AG04-p177
EXPNO 2
PROCNO 1
Date_ 20100519
Time 18.13
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 574.7
DW 62.400 use
DE 6.00 use
TE 293.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 =======
NUC1 1H
P1 12.80 use
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 ppm
2.02
1.96
2.20
2.27
1.02
4.51
2.15
0.99
3.58
2.38
3.59
1.07
3.23
2.97
3.00

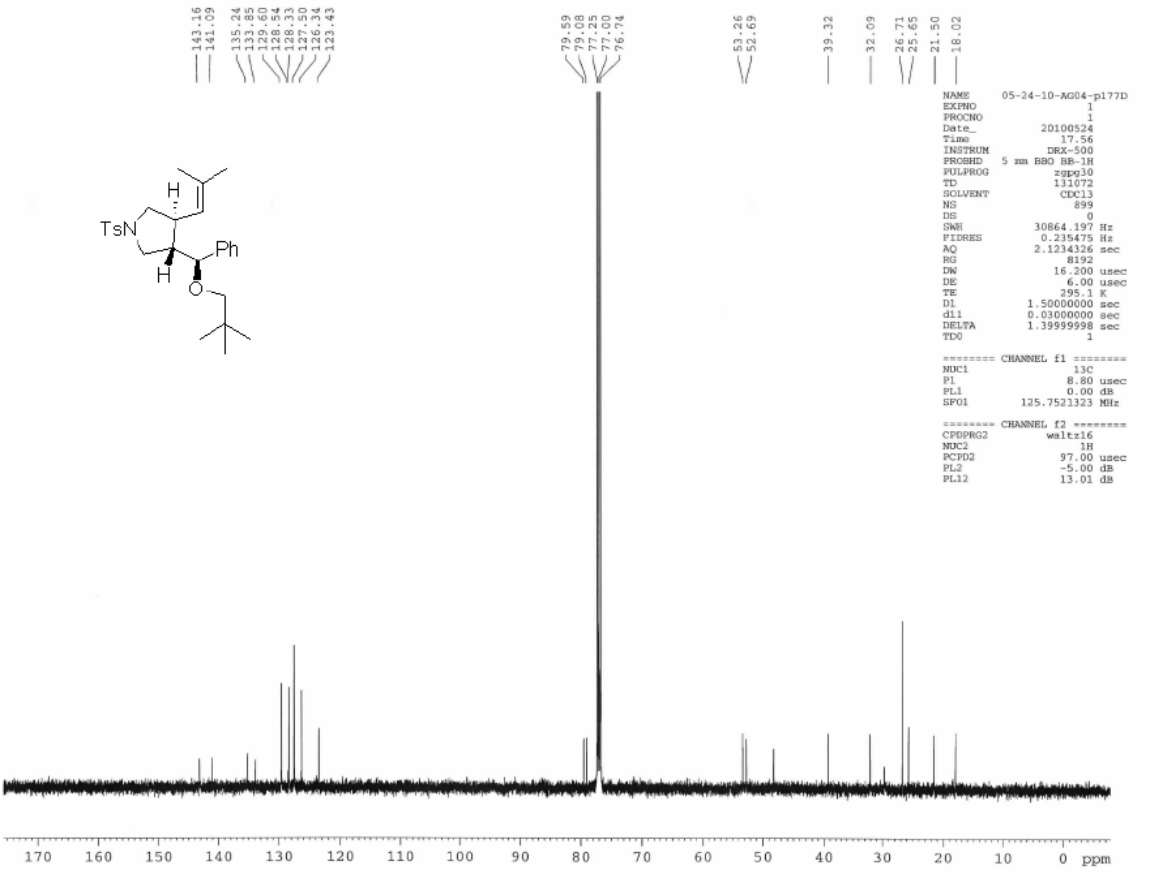

7.703
7.683
7.334
7.313
7.286
7.269
7.098
7.077
4.542
4.518
3.869
3.854
3.484
3.461
3.443
3.421
3.399
3.227
3.202
3.181
3.114
2.798
2.775
2.756
2.714
2.691
2.668
2.446
1.929
1.909
1.893
1.509
1.408
TsN
H
H
OMe
Cl
NAME 03-22-10-AG04-97C-
EXPNO 2
PROCNO 1
Date_ 20100322
Time 15.53
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 812.7
DW 62.400 use
DE 6.00 use
TE 292.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 =======
NUC1 1H
P1 12.80 use
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
0.14
2.25
2.09
1.70
2.15
1.15
1.13
2.29
1.17
2.95
2.40
3.22
1.18
3.03
3.00

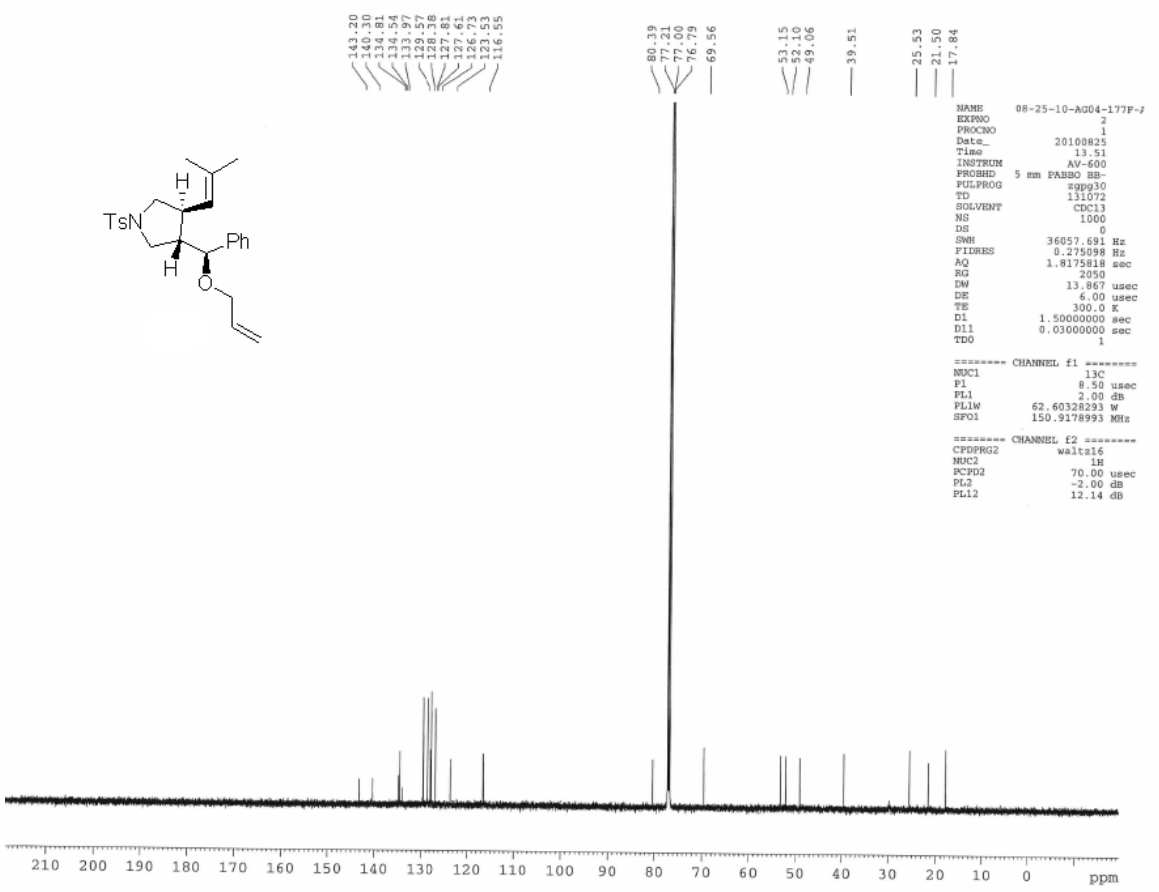

143.26
138.72
134.99
134.01
133.59
129.38
128.57
128.12
127.63
82.61
77.21
77.00
76.79
56.78
53.10
51.93
48.97
39.57
26.10
21.80
18.30
TsN
H
H
OMe
Cl
NAME 08-24-10-AG04-202
EXPNO 2
PROCNO 1
Date_ 20100824
Time 18.30
INSTRUM AV-600
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 782
DS 0
SWH 36057.691 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 13.867 usec
DE 6.00 usec
TE 301.0 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 2.00 dB
PL1W 62.60328293 W
SFO1 150.9178993 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -2.00 dB
PL12 12.14 dB
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

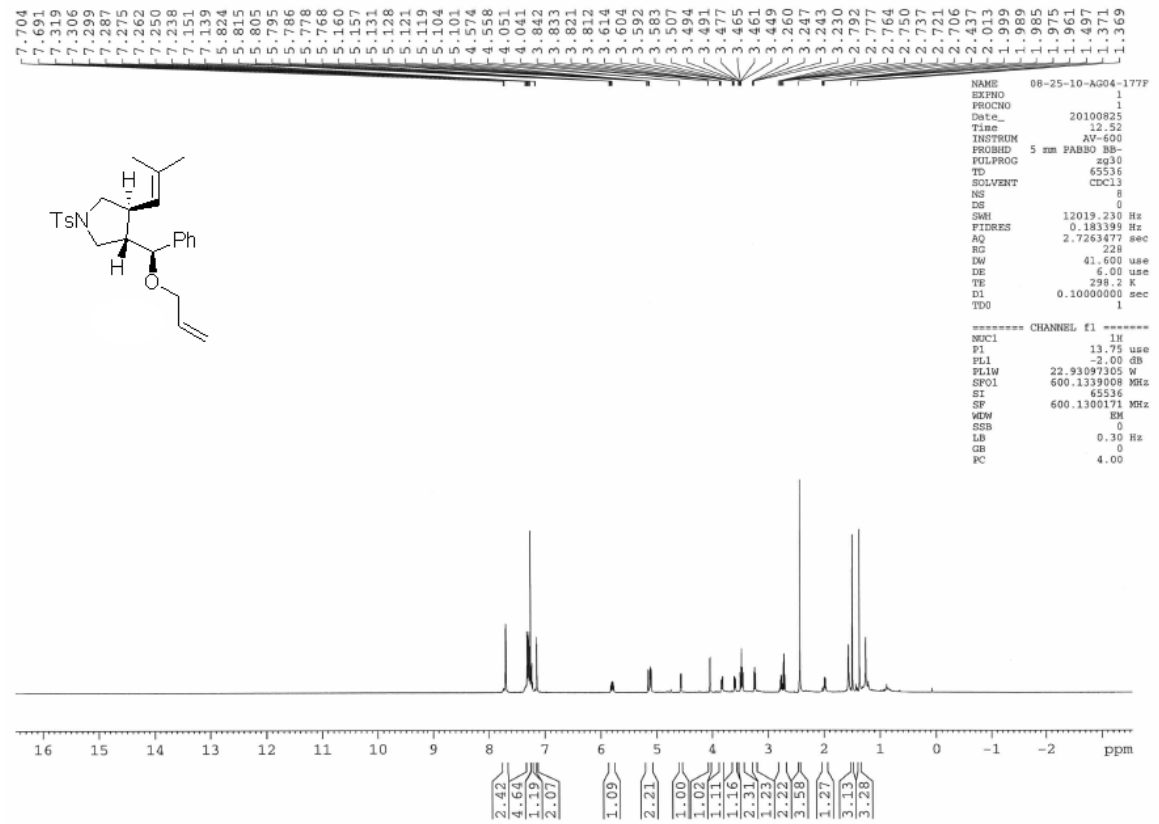

7.703
7.689
7.317
7.303
7.292
7.280
7.268
7.262
7.238
7.226
7.147
7.135
4.580
4.564
3.975
3.965
3.513
3.499
3.496
3.486
3.482
3.474
3.470
3.458
3.328
3.325
3.317
3.313
3.301
3.289
3.212
3.198
3.195
3.181
3.154
3.142
3.131
3.127
3.119
3.115
3.104
2.804
2.789
2.776
2.761
2.725
2.710
2.694
2.433
1.510
1.386
1.384
TsN
H
Ph
H
OEt
NAME 08-25-10-AG04-177B
EXPNO 1
PROCNO 1
Date_ 20100825
Time 12.00
INSTRUM AV-600
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 0
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 128
DW 41.600 use
DE 6.00 use
TE 297.1 K
D1 0.10000000 sec
TD0 1
======== CHANNEL f1 =======
NUC1 1H
P1 13.75 use
PL1 -2.00 dB
PL1W 22.93097305 W
SFO1 600.1339008 MHz
SI 65536
SF 600.1300171 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
2.11
4.13
1.03
2.00
1.00
1.04
2.14
1.13
1.10
1.15
1.05
1.05
3.36
1.05
3.08
3.02
3.36


143.16
140.93
134.81
134.07
129.53
128.31
127.63
127.60
126.59
123.56
80.66
77.21
77.00
76.79
64.30
53.18
52.15
48.92
39.47
25.54
21.49
17.79
15.14
TsN
H
Ph
H
OEt
NAME 08-25-10-AG04-177B-
EXPNO 2
PROCNO 1
Date_ 20100825
Time 12.49
INSTRUM AV-600
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 131072
SOLVENT CDC13
NS 835
DS 0
SWH 36057.691 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 13.867 usec
DE 6.00 usec
TE 299.8 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 2.00 dB
PL1W 62.60328293 W
SFO1 150.9178993 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -2.00 dB
PL12 12.14 dB
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.707
7.679
7.314
7.285
7.252
7.221
7.120
7.098
4.684
4.656
3.962
3.948
3.491
3.482
3.473
3.459
3.428
3.228
3.201
3.169
2.926
2.898
2.821
2.791
2.775
2.763
2.744
2.701
2.674
2.420
1.942
1.928
1.915
1.900
1.580
1.571
1.438
0.820
TsN
Ph
H
H
O
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 ppm
2.029
5.373
2.084
0.870
1.000
1.712
0.908
0.878
1.764
1.105
2.976
0.884
3.719
3.095
7.936


143.16
141.09
135.24
133.85
129.60
128.54
128.33
127.50
126.34
123.43
79.59
79.08
77.25
77.00
76.74
53.26
52.69
39.32
32.09
26.71
25.65
21.50
18.02
TsN
Ph
H
H
O
NAME 05-24-10-AG04-p177D
EXPNO 1
PROCNO 1
Date_ 20100524
Time 17.56
INSTRUM DRX-500
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 899
DS 0
SWH 30864.197 Hz
FIDRES 0.235475 Hz
AQ 2.1234326 sec
RG 8192
DW 16.200 usec
DE 6.00 usec
TE 295.1 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.80 usec
PL1 0.00 dB
SFO1 125.7521323 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 97.00 usec
PL2 -5.00 dB
PL12 13.01 dB
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


143.20
140.30
134.81
133.64
133.27
129.57
128.38
127.81
127.61
126.73
123.53
116.55
80.39
77.21
77.00
76.79
69.56
53.15
52.10
49.06
39.51
25.53
21.50
17.84
TsN
H
Ph
H
O
NAME 08-25-10-AG04-177F-
EXPNO 2
PROCNO 1
Date_ 20100825
Time 13.51
INSTRUM AV-600
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 1000
DS 0
SWH 36057.691 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 13.867 usec
DE 6.00 usec
TE 300.0 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 2.00 dB
PL1W 62.60328293 W
SFO1 150.9178993 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -2.00 dB
PL12 12.14 dB
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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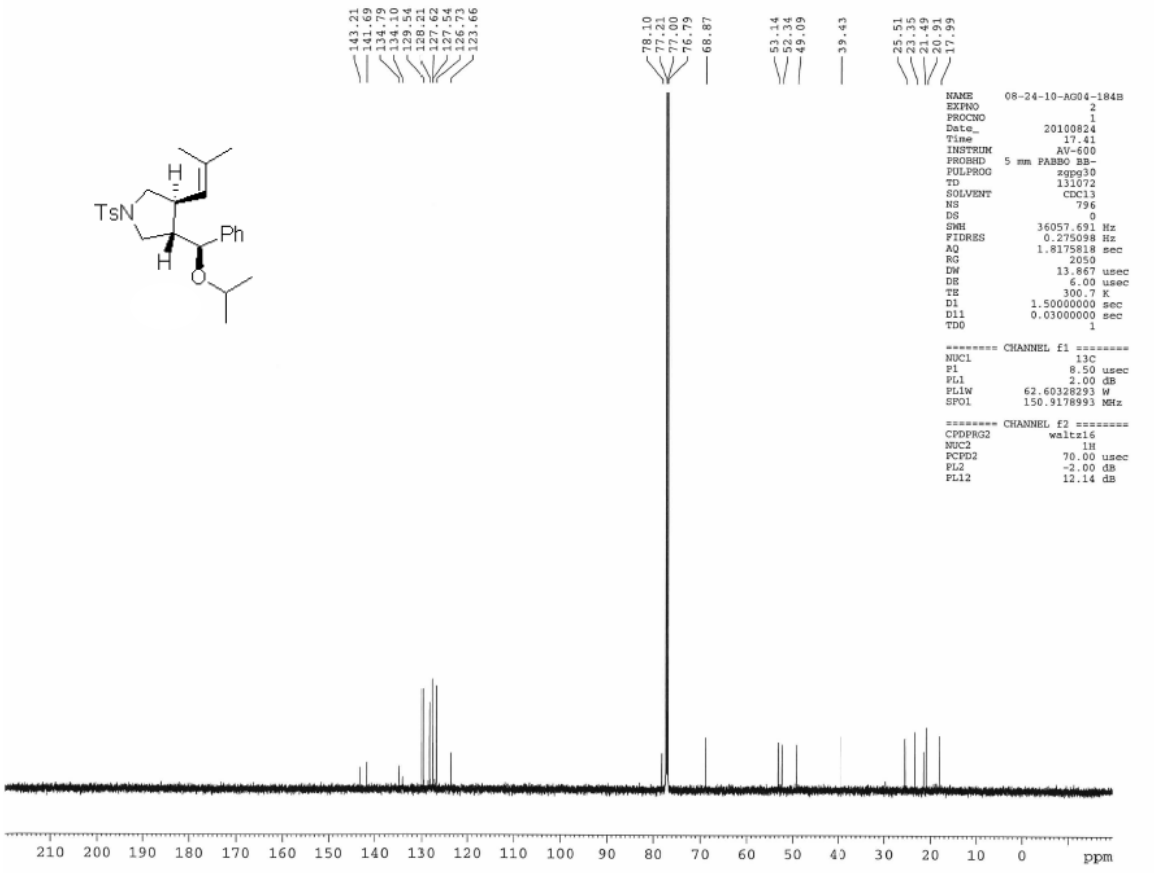
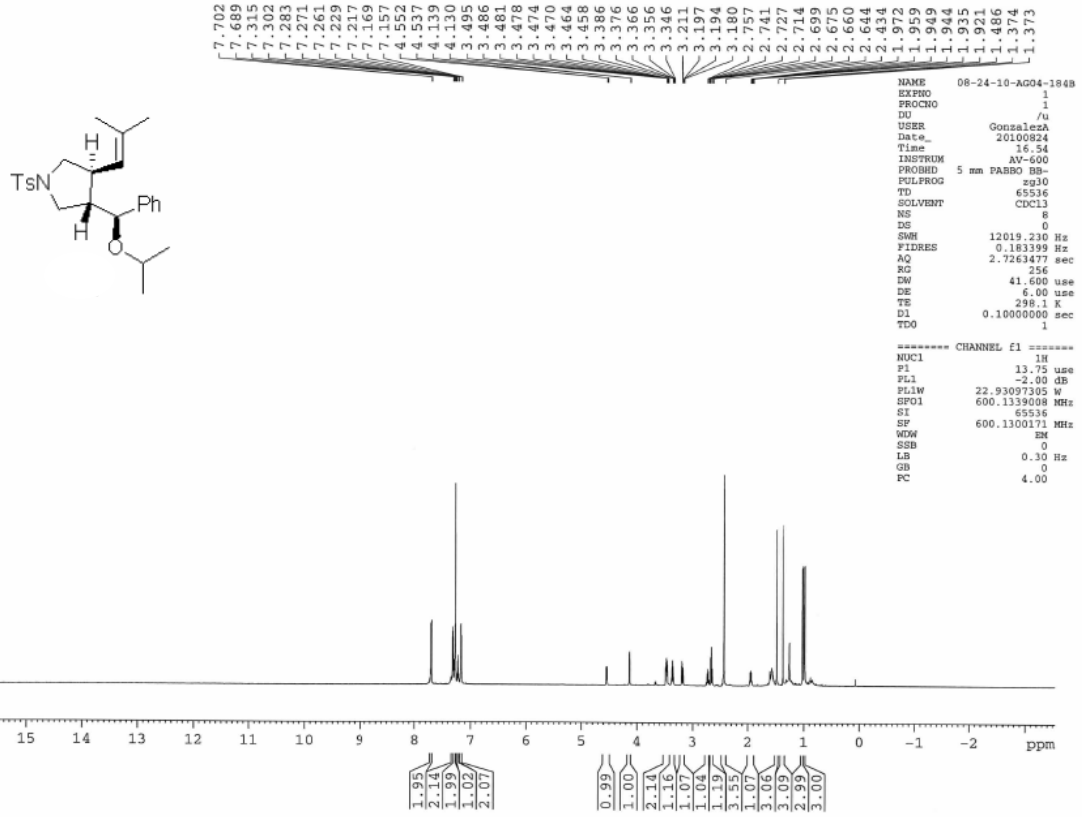
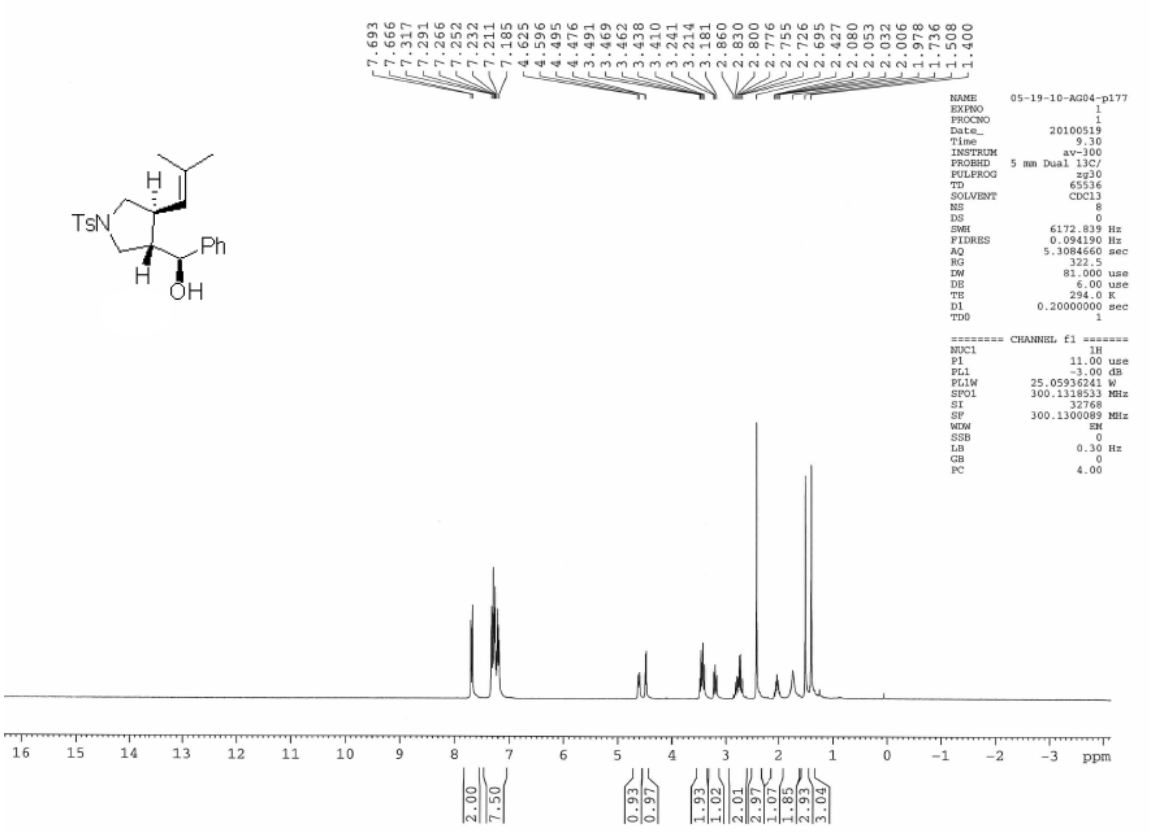
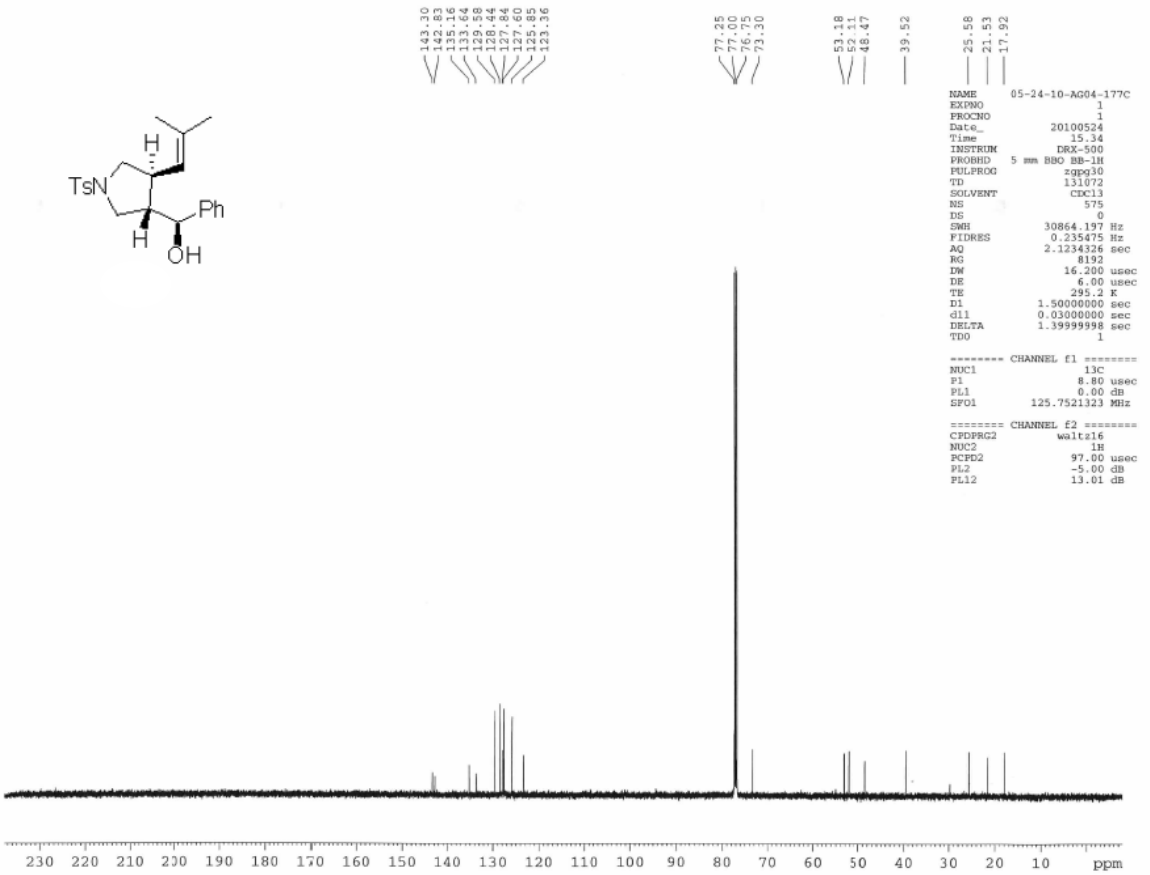
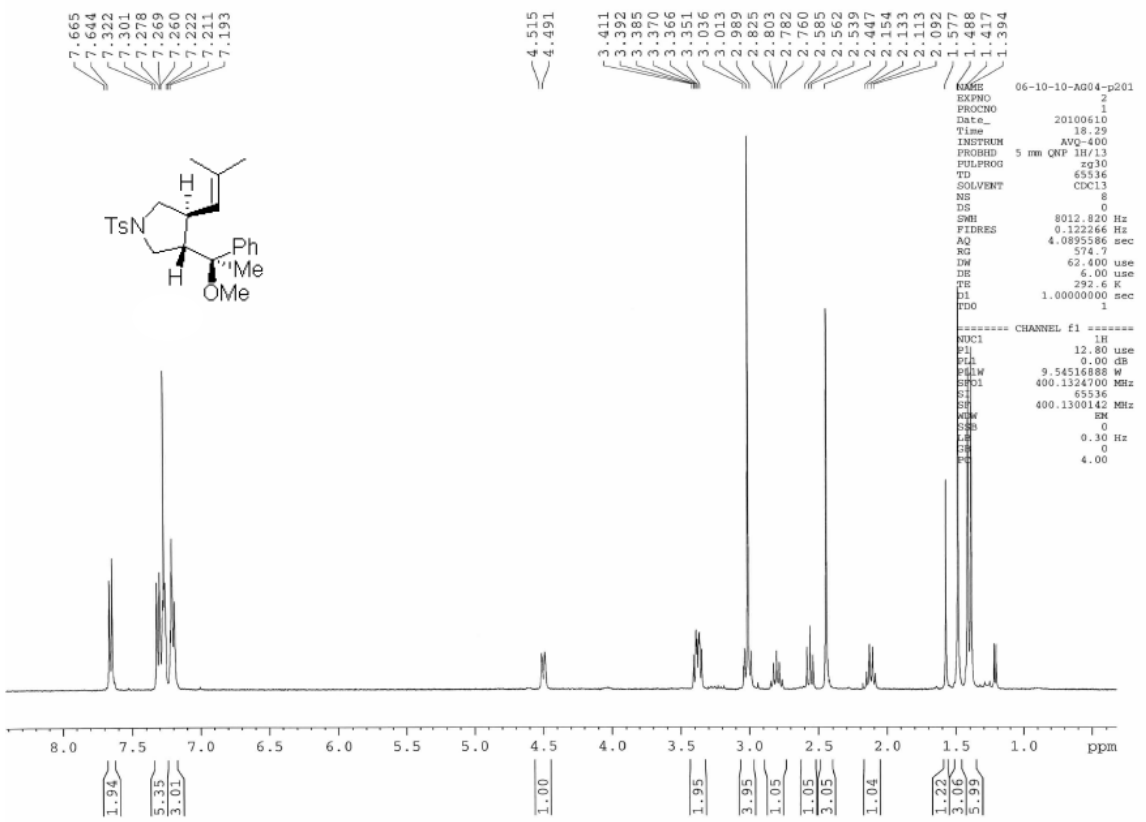
7.319
7.306
7.299
7.287
7.275
7.262
7.250
7.238
7.151
7.139
5.824
5.815
5.805
5.795
5.786
5.778
5.768
5.160
5.157
5.131
5.128
5.121
5.119
5.104
5.101
4.574
4.558
4.051
4.041
3.842
3.833
3.821
3.812
3.614
3.604
3.592
3.583
3.507
3.494
3.491
3.477
3.465
3.461
3.449
3.260
3.247
3.243
3.230
2.792
2.777
2.764
2.750
2.737
2.721
2.706
2.437
2.013
1.999
1.989
1.985
1.975
1.961
1.497
1.371
1.369
TsN
H
Ph
H
O
NAME 08-25-10-AG04-177F
EXPNO 1
PROCNO 1
Date_ 20100825
Time 12.52
INSTRUM AV-600
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 228
DW 41.600 use
DE 6.00 use
TE 298.2 K
D1 0.10000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.75 use
PL1 -2.00 dB
PL1W 22.93097305 W
SFO1 600.1339008 MHz
SI 65536
SF 600.1300171 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
2.42
4.64
1.19
2.07
1.09
2.21
1.00
1.02
1.11
1.16
2.31
1.23
2.22
3.58
1.27
3.13
3.28

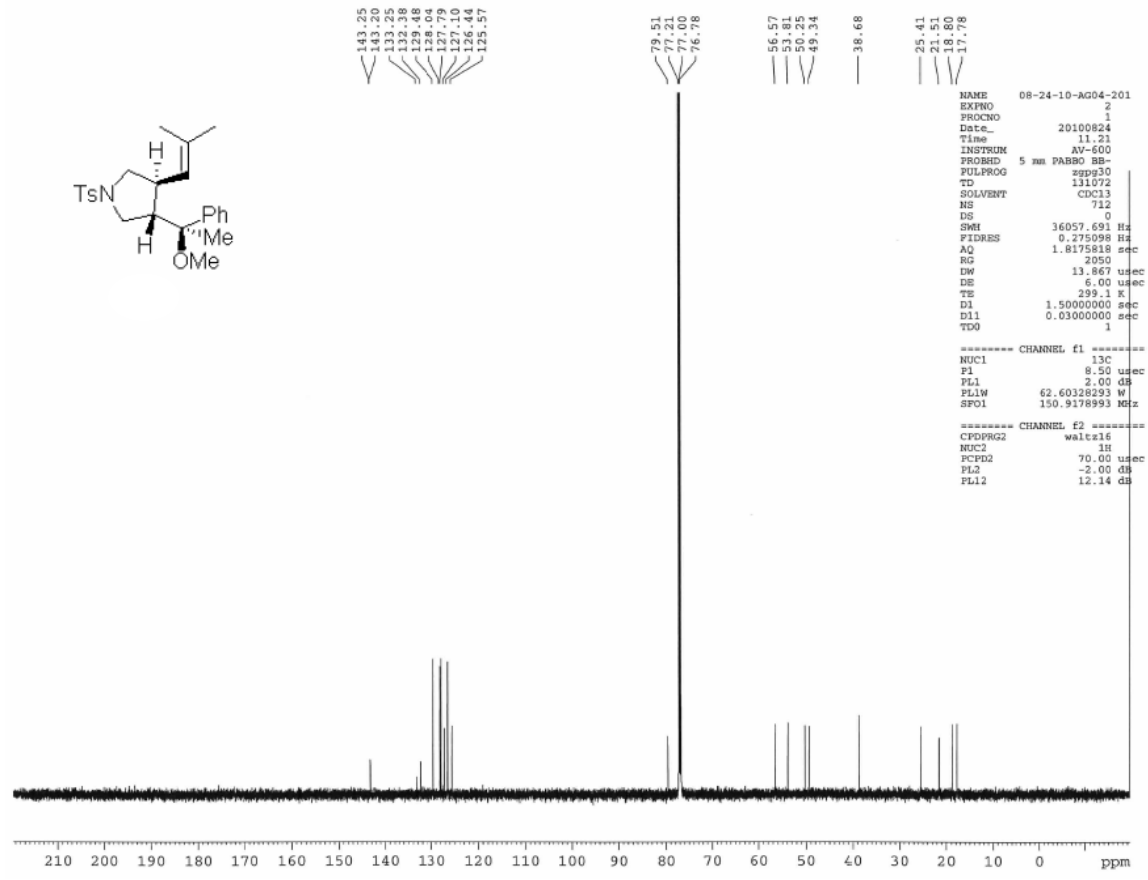

143.21
141.69
134.79
134.10
129.54
128.21
127.62
127.54
126.73
123.66
78.10
77.21
77.00
76.79
68.87
53.14
52.34
49.09
39.43
25.51
23.35
21.49
20.91
17.99
TsN
Ph
H
H
O
NAME 08-24-10-AG04-184B
EXPNO 2
PROCNO 1
Date_ 20100824
Time 17.41
INSTRUM AV-600
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 796
DS 0
SWH 36057.691 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 13.867 usec
DE 6.00 usec
TE 300.7 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 2.00 dB
PL1W 62.60328293 W
SFO1 150.9178993 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -2.00 dB
PL12 12.14 dB
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

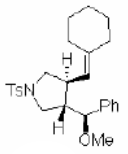

7.702
7.689
7.315
7.302
7.283
7.271
7.261
7.229
7.217
7.169
7.157
4.552
4.537
4.139
4.130
3.495
3.486
3.481
3.478
3.474
3.470
3.464
3.458
3.386
3.376
3.366
3.356
3.346
3.211
3.197
3.194
3.180
2.757
2.741
2.727
2.714
2.699
2.675
2.660
2.644
2.634
1.972
1.959
1.949
1.944
1.935
1.921
1.486
1.374
1.373
TsN
Ph
H
H
O
NAME 08-24-10-AG04-184B
EXPNO 1
PROCNO 1
DU /u
USER GonzalezA
Date_ 20100824
Time 16.54
INSTRUM AV-600
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 256
DW 41.600 use
DE 6.00 use
TE 298.1 K
D1 0.10000000 sec
TD0 1
======== CHANNEL f1 =======
NUC1 1H
P1 13.75 use
PL1 -2.00 dB
PL1W 22.93097305 W
SFO1 600.1339008 MHz
SI 65536
SF 600.1300171 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.95
2.14
1.99
1.02
2.07
0.99
1.00
2.14
1.16
1.07
1.04
1.19
3.55
1.07
3.06
3.09
2.99
3.00

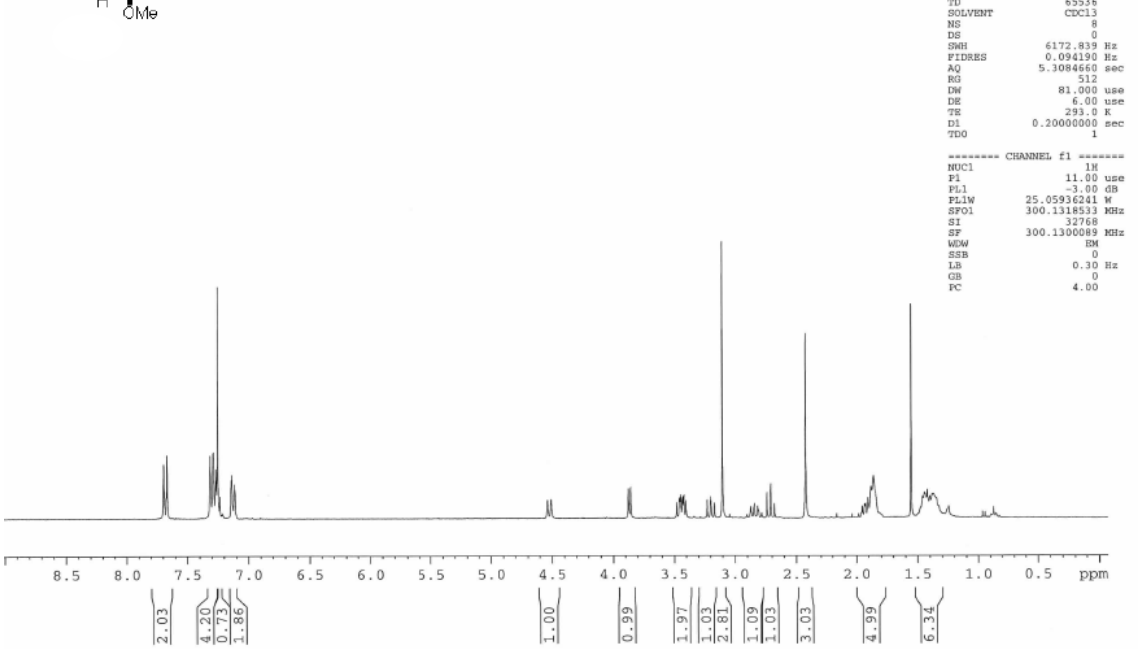

7.693
7.666
7.317
7.291
7.266
7.252
7.232
7.211
7.185
4.625
4.596
4.495
4.476
3.491
3.469
3.462
3.438
3.410
3.241
3.214
3.181
2.860
2.830
2.800
2.776
2.755
2.726
2.695
2.427
2.080
2.053
2.032
2.006
1.978
1.736
1.508
1.400
TsN
H
Ph
H
OH
NAME 05-19-10-AG04-p177
EXPNO 1
PROCNO 1
Date_ 20100519
Time 9.30
INSTRUM av-300
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 322.5
DW 81.000 use
DE 6.00 use
TE 294.0 K
D1 0.20000000 sec
TD0 1
======== CHANNEL f1 =======
NUC1 1H
P1 11.00 use
PL1 -3.00 dB
PL1W 25.05936241 W
SFO1 300.1318533 MHz
SI 32768
SF 300.1300089 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 ppm
2.00
7.50
0.93
0.97
1.93
1.02
2.01
2.97
1.07
1.85
2.93
3.04

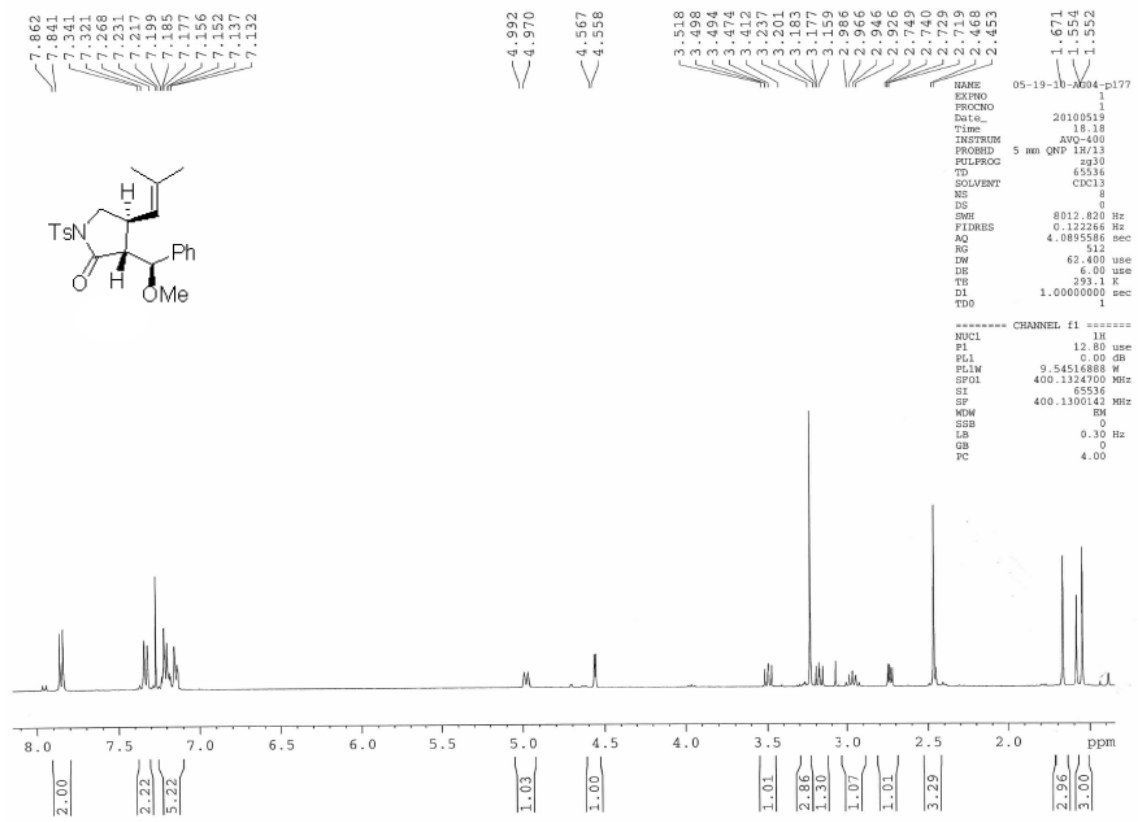

143.30
142.83
135.16
133.64
129.58
128.44
127.84
127.60
125.55
123.56
77.25
77.00
76.75
73.30
53.18
52.11
48.47
39.52
25.58
21.53
17.92
TsN
H
Ph
H
OH
NAME 05-24-10-AG04-177C
EXPNO 1
PROCNO 1
Date_ 20100524
Time 15.34
INSTRUM DRX-500
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 575
DS 0
SWH 30864.197 Hz
FIDRES 0.235475 Hz
AQ 2.1234326 sec
RG 8192
DW 16.200 usec
DE 6.00 usec
TE 295.2 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.80 usec
PL1 0.00 dB
SFO1 125.7521323 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 97.00 usec
PL2 -5.00 dB
PL12 13.01 dB
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.665
7.644
7.322
7.301
7.278
7.269
7.260
7.222
7.211
7.193
4.515
4.491
3.411
3.392
3.385
3.370
3.366
3.351
3.036
3.013
2.989
2.825
2.803
2.782
2.760
2.585
2.562
2.539
2.447
2.154
2.133
2.113
2.092
1.577
1.488
1.417
1.394
TsN
H
Ph
Me
H
OMe
NAME 06-10-10-AG04-p201
EXPNO 2
PROCNO 1
Date_ 20100610
Time 18.29
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 574.7
DW 62.400 use
DE 6.00 use
TE 292.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 =======
NUC1 1H
P1 12.80 use
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.94
5.35
3.01
1.00
1.95
3.95
1.05
1.05
3.05
1.04
1.22
3.06
5.99

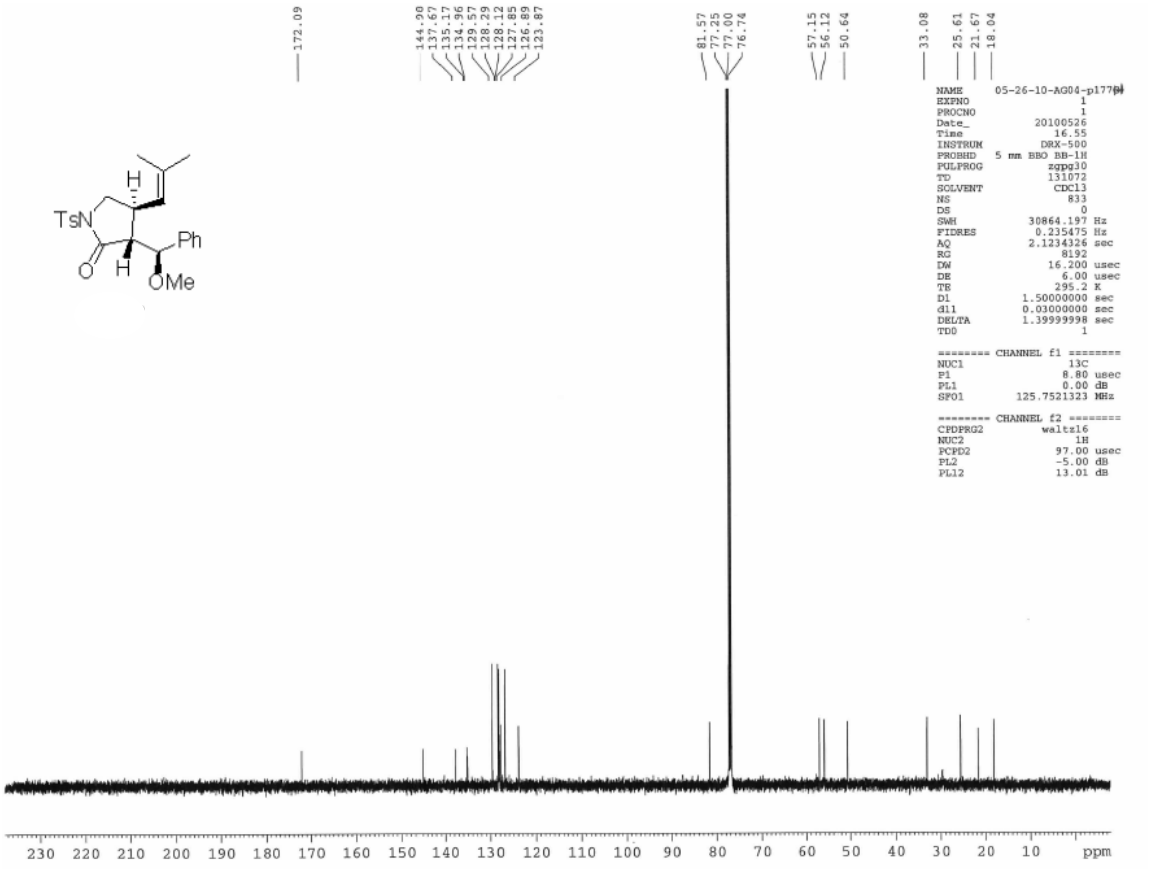

143.25
143.20
133.25
132.38
129.48
128.04
127.79
127.10
126.44
125.57
79.51
77.21
77.00
76.78
56.57
53.81
50.25
49.34
38.68
25.41
21.51
18.80
17.78
TsN
H
Ph
Me
H
OMe
NAME 08-24-10-AG04-201
EXPNO 2
PROCNO 1
Date_ 20100824
Time 11.21
INSTRUM AV-600
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 712
DS 0
SWH 36057.691 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 13.867 usec
DE 6.00 usec
TE 299.1 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 =======
NUC1 13C
P1 8.50 usec
PL1 2.00 dB
PL1W 62.60328293 W
SFO1 150.9178993 MHz
======== CHANNEL f2 =======
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -2.00 dB
PL12 12.14 dB
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

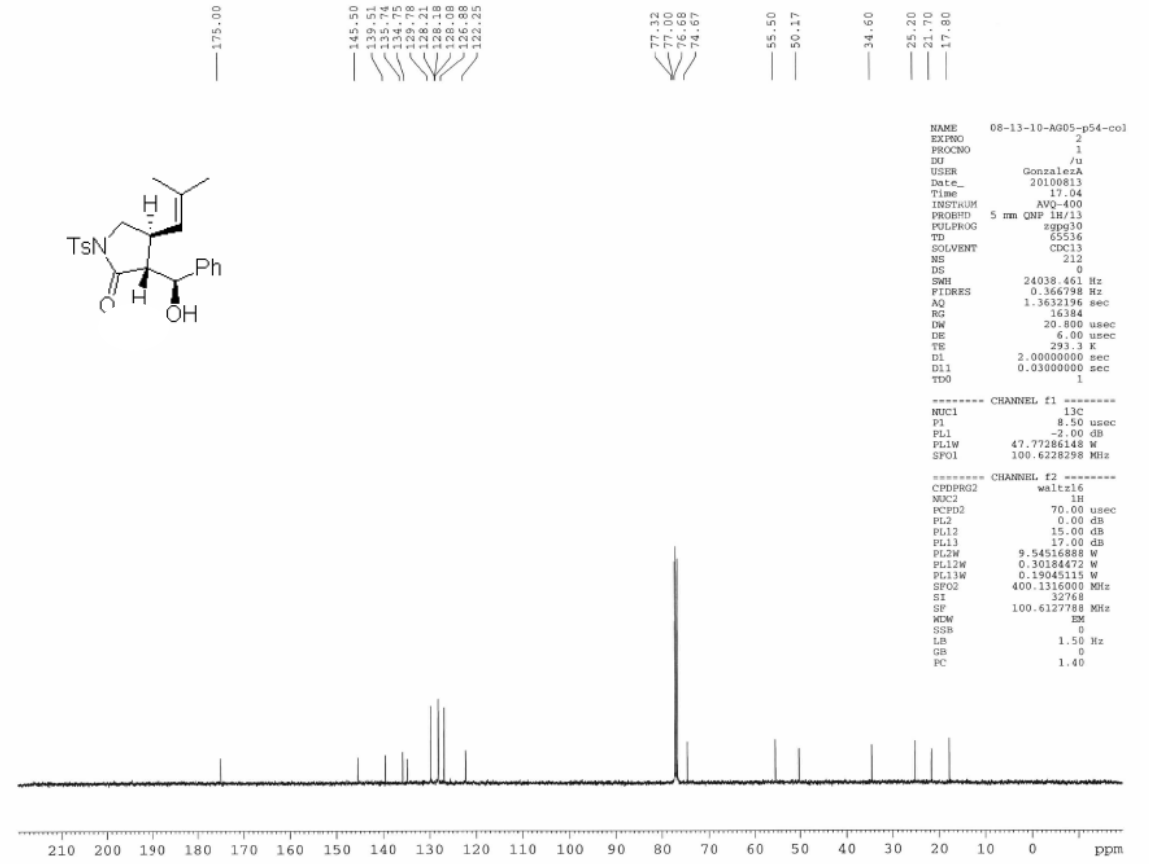

H
TsN
Ph
H
OMe

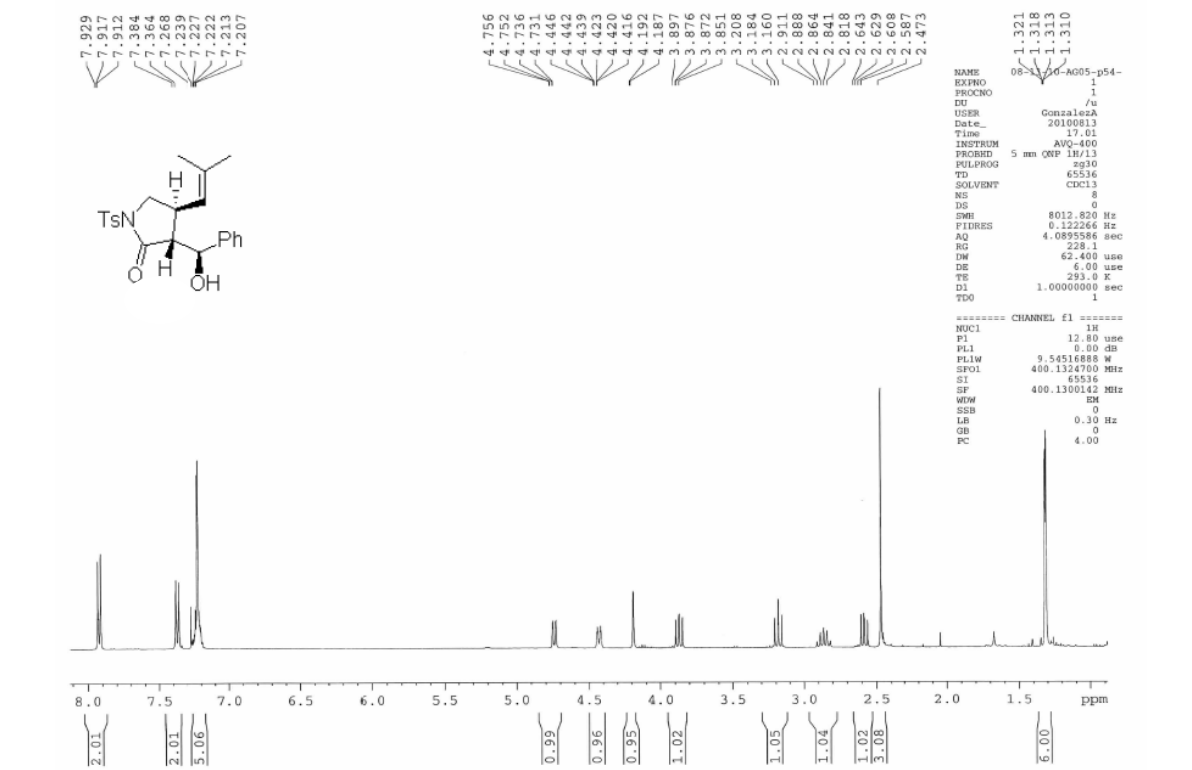

NAME 06-14-10-AG04-p208
EXPNO 1
PROCNO 1
Date_ 20100614
Time 14.55
INSTRUM av-300
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 512
DW 81.000 use
DE 6.00 use
TE 293.0 K
D1 0.20000000 sec
TD0 1
======== CHANNEL f1 =======
NUC1 1H
P1 11.00 use
PL1 -3.00 dB
PL1W 25.05936241 W
SFO1 300.1318533 MHz
SI 32768
SF 300.1300089 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.03 4.20 0.73 1.86 1.00 0.99 1.97 1.03 2.81 1.09 1.03 3.03 4.99 6.34

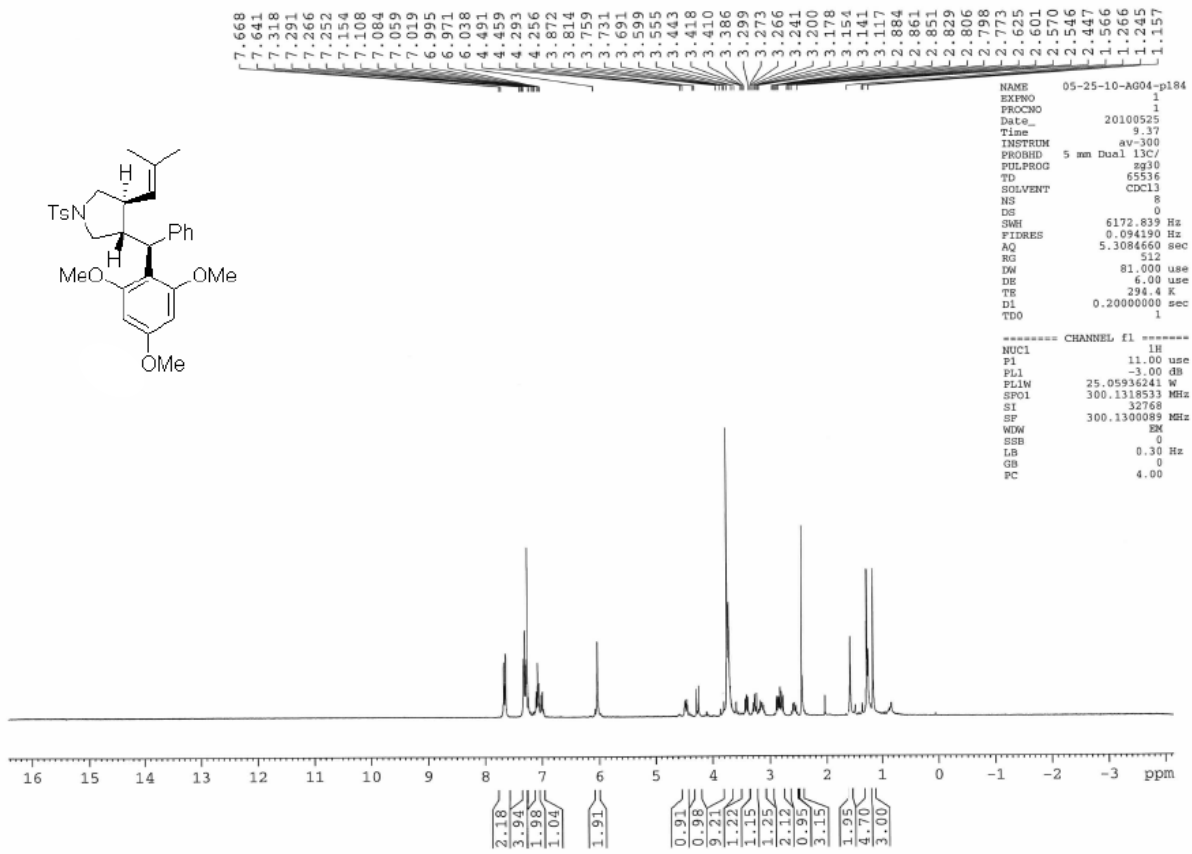

7.862 7.841 7.341 7.321 7.268 7.231 7.217 7.199 7.185 7.177 7.156 7.152 7.137 7.132
4.992 4.970 4.567 4.558
3.518 3.498 3.494 3.474 3.412 3.237 3.201 3.183 3.177 3.159 2.986 2.966 2.946 2.926 2.749 2.740 2.729 2.719 2.468 2.453
1.671 1.554 1.552
NAME 05-19-10-AG04-p177
EXPNO 1
PROCNO 1
Date_ 20100519
Time 18.18
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 512
DW 62.400 use
DE 6.00 use
TE 293.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 =======
NUC1 1H
P1 12.80 use
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 ppm
2.00 2.22 5.22 1.03 1.00 1.01 2.86 1.30 1.07 1.01 3.29 2.96 3.00

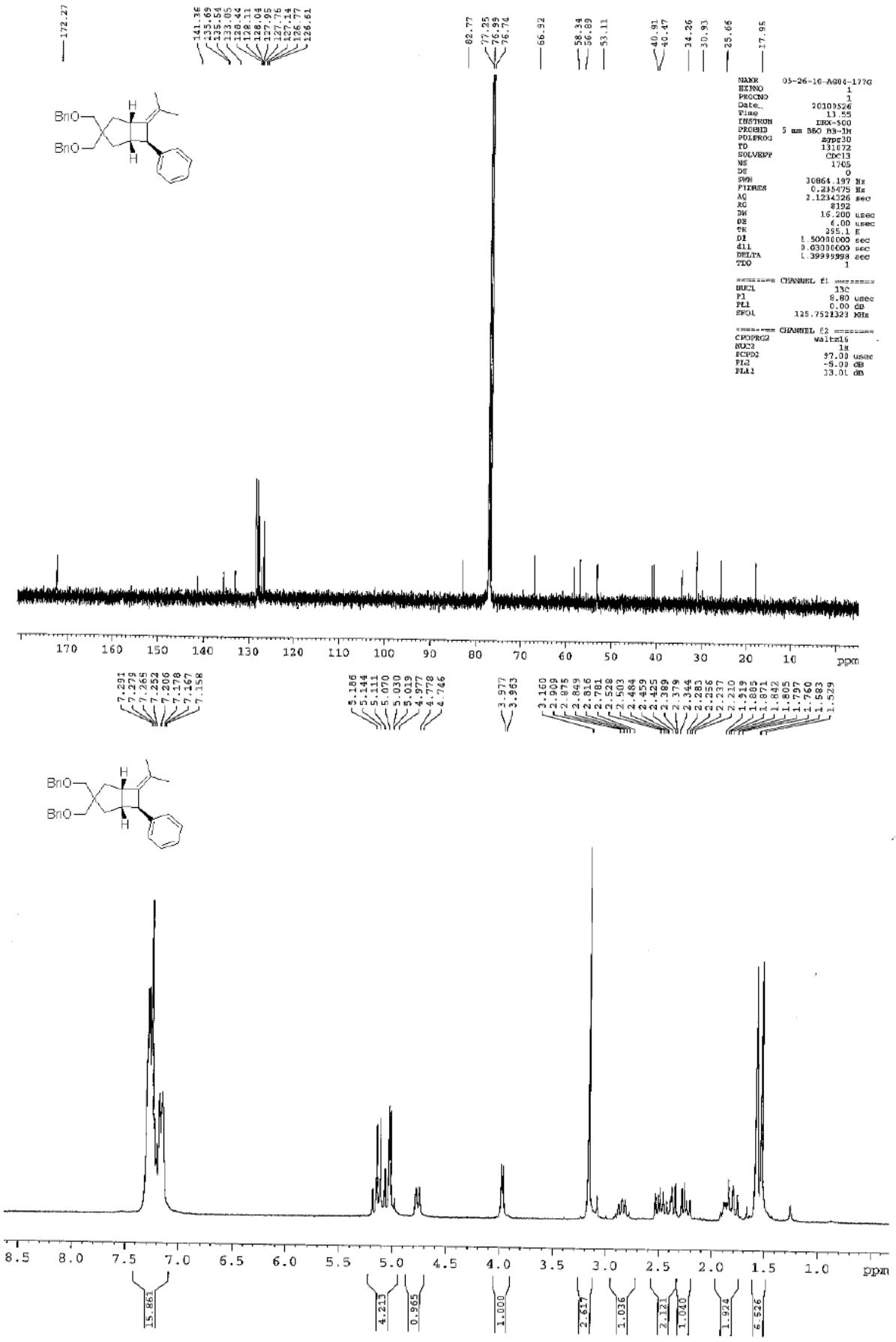
H
TsN
O
H
Ph
OMe

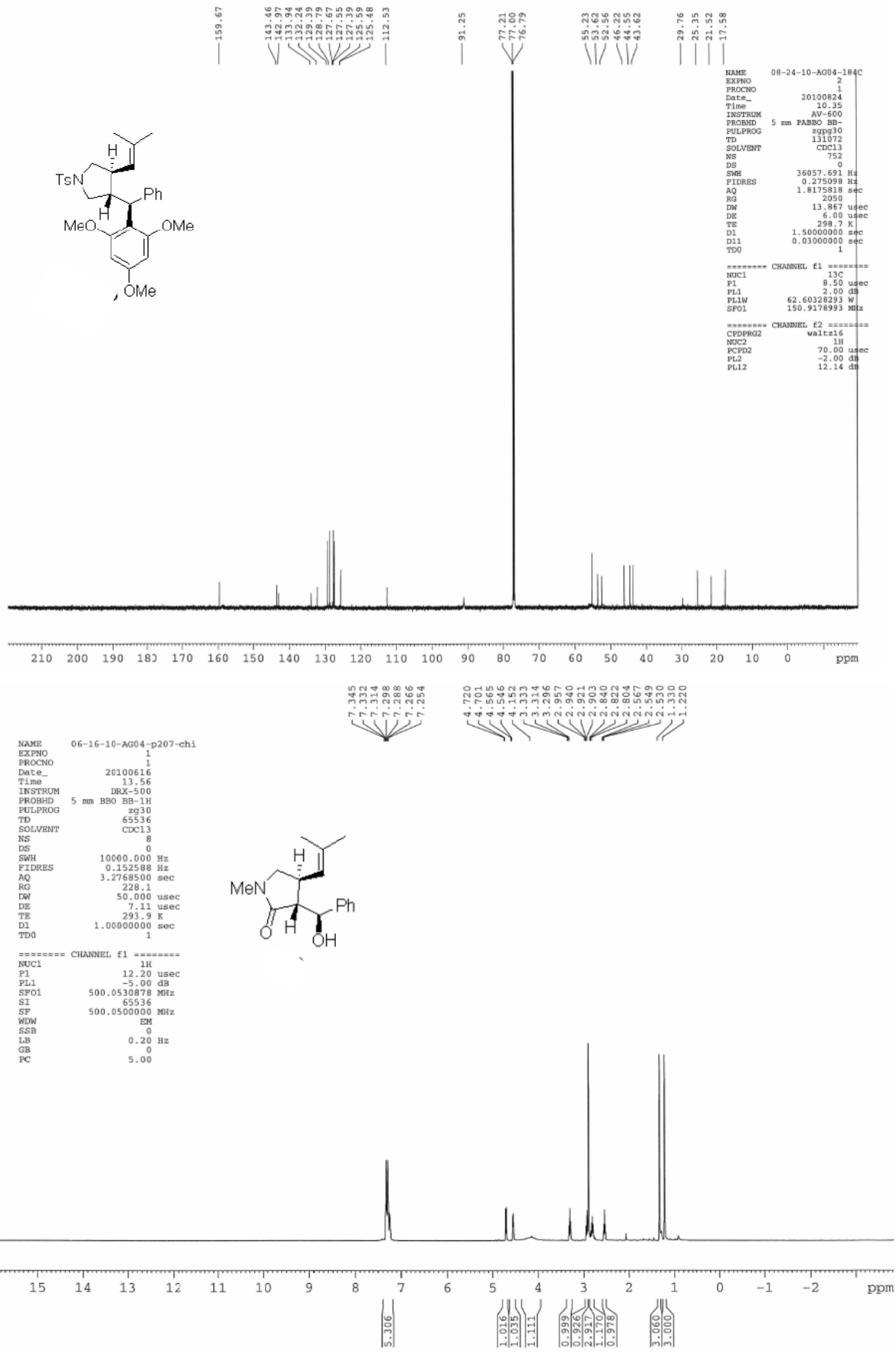

172.09
144.90
137.67
135.17
134.96
129.57
128.29
128.12
127.85
126.89
123.87
81.57
77.25
77.00
76.74
57.15
56.12
50.64
33.08
25.61
21.67
18.04
TsN
H
Ph
O
H
OMe
NAME 05-26-10-AG04-p177
EXPNO 1
PROCNO 1
Date_ 20100526
Time 16.55
INSTRUM DRX-500
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 833
DS 0
SWH 30864.197 Hz
FIDRES 0.235475 Hz
AQ 2.1234326 sec
RG 8192
DW 16.200 usec
DE 6.00 usec
TE 295.2 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.80 usec
PL1 0.00 dB
SFO1 125.7521323 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 97.00 usec
PL2 -5.00 dB
PL12 13.01 dB
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

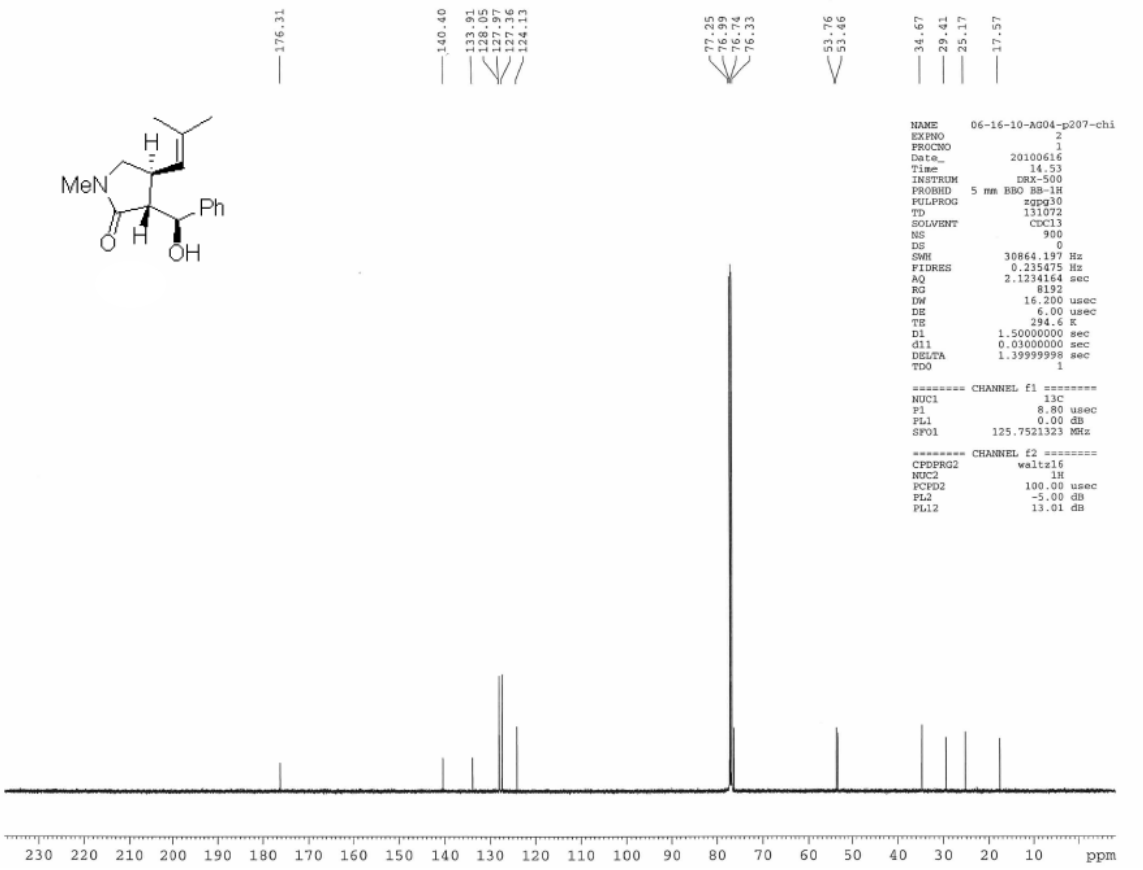

175.00
145.50
139.51
135.74
134.75
129.78
128.21
128.18
128.08
126.88
122.25
77.32
77.00
76.68
74.67
55.50
50.17
34.60
25.20
21.70
17.80
TsN
H
Ph
O
H
OH
NAME 08-13-10-AG05-p54-col
EXPNO 2
PROCNO 1
DU /u
USER GonzalezA
Date_ 20100813
Time 17.04
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 212
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3632196 sec
RG 16384
DW 20.800 usec
DE 6.00 usec
TE 293.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 -2.00 dB
PL1W 47.77286148 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 17.00 dB
PL2W 9.54516888 W
PL12W 0.30184472 W
PL13W 0.19045115 W
SFO2 400.1316000 MHz
SI 32768
SF 100.6127788 MHz
WDW EM
SSB 0
LB 1.50 Hz
GB 0
PC 1.40
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

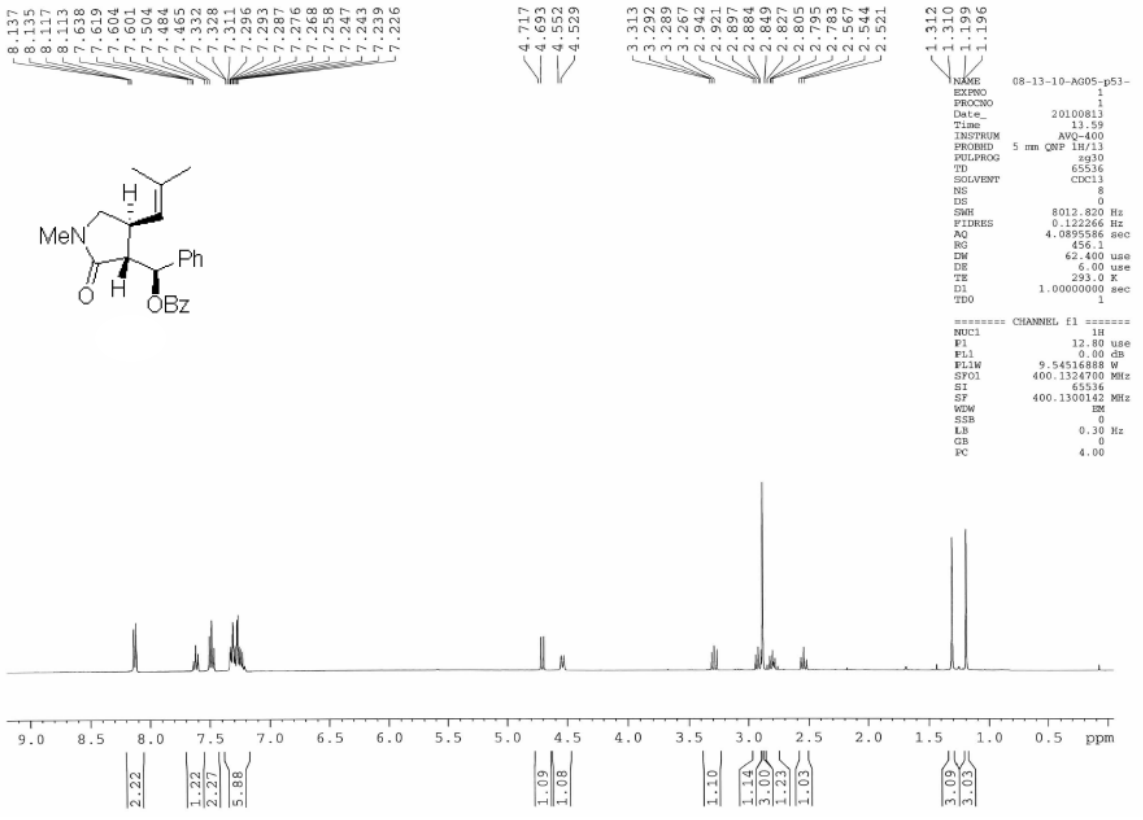

TsN
Ph
H
O
OH
NAME 08-13-10-AG05-p54-
EXPNO 1
PROCNO 1
DU /u
USER GonzalezA
Date_ 20100813
Time 17.01
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 228.1
DW 62.400 use
DE 6.00 use
TE 293.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 =======
NUC1 1H
P1 12.80 use
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
ppm

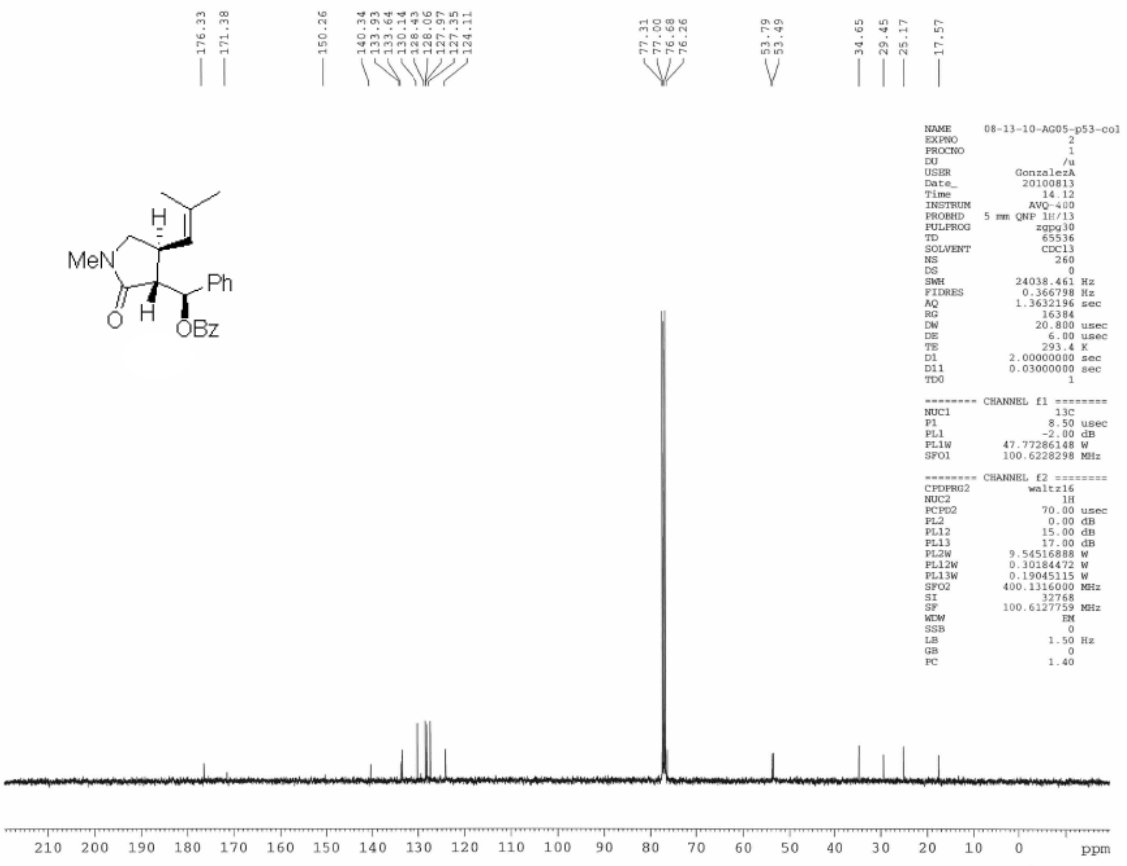

TsN
Ph
H
MeO
OMe
OMe
NAME 05-25-10-AG04-p184
EXPNO 1
PROCNO 1
Date_ 20100525
Time 9.37
INSTRUM av-300
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 512
DW 81.000 use
DE 6.00 use
TE 294.4 K
D1 0.20000000 sec
TD0 1
======== CHANNEL f1 =======
NUC1 1H
P1 11.00 use
PL1 -3.00 dB
PL1W 25.05936241 W
SFO1 300.1318533 MHz
SI 32768
SF 300.1300089 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
ppm


BnO
BnO
H
H
172.27
141.36
135.69
135.54
133.05
128.44
128.11
128.01
127.95
127.76
127.14
126.77
126.61
82.77
77.25
76.99
76.74
66.92
58.34
56.89
53.11
40.91
40.47
34.26
30.93
25.65
17.95
ppm
7.291
7.279
7.265
7.252
7.206
7.178
7.167
7.158
5.186
5.144
5.111
5.070
5.030
5.019
4.977
4.778
4.746
3.977
3.963
3.160
2.909
2.875
2.849
2.816
2.781
2.528
2.503
2.484
2.459
2.425
2.389
2.379
2.344
2.281
2.256
2.237
2.210
1.919
1.885
1.871
1.842
1.805
1.797
1.760
1.583
1.529
15.863
4.213
0.965
1.000
2.817
1.036
2.121
1.040
1.924
6.526


159.67
143.46
142.97
133.94
132.24
129.39
128.79
127.67
127.55
127.39
126.59
125.48
112.53
91.25
77.21
77.00
76.79
55.23
53.62
52.56
46.22
46.55
43.62
29.76
25.35
21.52
17.58
TsN
Ph
MeO
OMe
OMe
NAME 08-24-10-AG04-184C
EXPNO 2
PROCNO 1
Date_ 20100824
Time 10.35
INSTRUM AV-600
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 752
DS 0
SWH 36057.691 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 13.867 usec
DE 6.00 usec
TE 298.7 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 2.00 dB
PL1W 62.60328293 W
SFO1 150.9178993 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -2.00 dB
PL12 12.14 dB
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
7.345
7.332
7.314
7.298
7.288
7.266
7.254
4.720
4.701
4.565
4.546
4.152
3.333
3.314
3.296
2.957
2.940
2.921
2.903
2.840
2.822
2.804
2.567
2.549
2.530
1.330
1.220
NAME 06-16-10-AG04-p207-chi
EXPNO 1
PROCNO 1
Date_ 20100616
Time 13.56
INSTRUM DRX-500
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2768500 sec
RG 228.1
DW 50.000 usec
DE 7.11 usec
TE 293.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.20 usec
PL1 -5.00 dB
SFO1 500.0530878 MHz
SI 65536
SF 500.0500000 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 5.00
MeN
Ph
O
H
OH
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
5.306
1.016
1.035
1.111
0.999
0.926
2.917
1.170
0.978
3.060
3.000


176.31
140.40
133.91
128.05
127.97
127.36
124.13
77.25
76.99
76.74
76.33
53.76
53.46
34.67
29.41
25.17
17.57
MeN
Ph
H
O
OH
NAME 06-16-10-AG04-p207-chi
EXPNO 2
PROCNO 1
Date_ 20100616
Time 14.53
INSTRUM DRX-500
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 900
DS 0
SWH 30864.197 Hz
FIDRES 0.235475 Hz
AQ 2.1234164 sec
RG 8192
DW 16.200 usec
DE 6.00 usec
TE 294.6 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.80 usec
PL1 0.00 dB
SFO1 125.7521323 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -5.00 dB
PL12 13.01 dB
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.137
8.135
8.117
8.113
7.638
7.619
7.604
7.601
7.504
7.484
7.465
7.332
7.328
7.311
7.296
7.293
7.287
7.276
7.268
7.258
7.247
7.243
7.239
7.226
4.717
4.693
4.552
4.529
3.313
3.292
3.289
3.267
2.942
2.921
2.897
2.884
2.849
2.827
2.805
2.795
2.783
2.567
2.544
2.521
1.312
1.310
1.199
1.196
MeN
Ph
H
O
OBz
NAME 08-13-10-AG05-p53-
EXPNO 1
PROCNO 1
Date_ 20100813
Time 13.59
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 456.1
DW 62.400 use
DE 6.00 use
TE 293.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 =======
NUC1 1H
P1 12.80 use
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.22
1.22
2.27
5.88
1.09
1.08
1.10
1.14
3.00
1.23
1.03
3.09
3.03


176.33
171.38
150.26
140.34
133.23
131.63
130.14
128.43
128.06
127.97
127.35
124.11
77.31
77.00
76.68
76.26
53.79
53.49
34.65
29.45
25.17
17.57
MeN
H
Ph
O
H
OBz
NAME 08-13-10-AG05-p53-col
EXPNO 2
PROCNO 1
DU /u
USER GonzalezA
Date_ 20100813
Time 14.12
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 260
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3632196 sec
RG 16384
DW 20.800 usec
DE 6.00 usec
TE 293.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 -2.00 dB
PL1W 47.77286148 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 17.00 dB
PL2W 9.54516888 W
PL12W 0.30184472 W
PL13W 0.19045115 W
SFO2 400.1316000 MHz
SI 32768
SF 100.6127759 MHz
WDW EM
SSB 0
LB 1.50 Hz
GB 0
PC 1.40
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

5. Computational Details

Calculations were performed using density functional theory (DFT) with the M06 functional, as implemented in Jaguar 7.6.[1] All calculations used the Hay and Wadt small core-valence relativistic effective-core-potential[2] (ECP). The LACVP** basis set was used for all geometry optimizations and LACV3P++**(2f) for energies. LACV3P++**(2f) utilizes the LACV3P++** basis set as implemented in Jaguar plus a double-zeta f-shell with exponents from Martin and Sundermann.[3] All electrons were described for all other atoms using the 6-31G** or 6-311++G** basis sets.[4,5] For each optimized structure, the M06 analytic Hessian was calculated to obtain the vibrational frequencies, which in turn were used to obtain the zero point energies and free energy corrections (without translational or rotational components). Solvent corrections were based on single point self-consistent Poisson-Boltzmann continuum solvation calculations for CH_2Cl_2 (e = 8.93 and R0= 2.33 Å) using the PBF[6] module in Jaguar.

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Reactant

C1	5.5889579340	12.4302859727	14.4642927992
H2	6.6477772238	12.3536594602	14.7298693523
C3	5.4846745330	9.9714618631	14.3129795373
H4	5.2151315398	9.1389799762	13.6590813759
N5	5.2350584223	11.2587470712	13.6469231186
O6	4.1654098094	12.7863465392	11.9623485383
O7	4.2988427829	10.2170603327	11.4244013650
P8	3.9685243209	11.3042435923	12.5600071605
Au9	1.7983109346	10.8195510367	13.3189058580
H10	6.5522183078	9.8935936080	14.5407449527
H11	4.9213249219	9.8793820969	15.2521591905
H12	5.0014438492	12.4771418004	15.3918966714
H13	5.4434386437	13.3470709927	13.8955361593
C14	3.1472550445	13.4306802281	11.1606517920
H15	2.9769830678	12.8745323994	10.2353916751
H16	3.5353589482	14.4223191542	10.9297905629
H17	2.2152888231	13.5207203442	11.7261769696
C18	5.5720838484	10.2118437045	10.7110599639
H19	6.3663479810	9.8495000708	11.3656471931
H20	5.8107200347	11.2140820745	10.3499603937
H21	5.4323507620	9.5313440088	9.8723442882
C22	0.0102947001	10.4789852333	14.7462823142
C23	-0.5896296349	10.3577093508	13.5355143861
C26	0.2943174946	10.5664285263	16.0284405792
H27	1.3175403430	10.7678388354	16.3395943688
C28	-0.7041257186	10.4169017213	17.1558740459
H29	-0.5972431404	11.3069251734	17.7892967114
H30	-1.7248469237	10.4190745271	16.7622197137
C31	-0.4810990412	9.1530818718	18.0185711884
H32	-1.1658413979	9.2184402134	18.8729151341
H33	-0.7812055560	8.2665264060	17.4477075987
C34	0.9618547685	8.9448386302	18.5320576792
H35	1.6181041619	8.6529909484	17.7019681420
H36	0.9435711209	8.0870214838	19.2190312297
C37	1.5437149321	10.1430512836	19.2317395502
H38	0.9534878822	10.5513567412	20.0522588330
C39	2.7195826580	10.7065720089	18.9097030973
H40	3.2938887971	10.2434669229	18.1034242395
C41	3.3695604344	11.8772419705	19.5202654068
C42	4.7112110306	14.1092201597	20.6048746594
C43	4.6595023042	12.2325581929	19.0880137750
C44	2.7641796127	12.6714871070	20.5115513344
C45	3.4284512586	13.7713098784	21.0456794520
C46	5.3259737801	13.3335994653	19.6226653153
H47	5.1501351894	11.6232450595	18.3314919515
H48	1.7670463152	12.4318008775	20.8673857829
H49	2.9443763590	14.3713165936	21.8109094497
H50	6.3257492434	13.5826165621	19.2772520053
H51	5.2255321274	14.9680751741	21.0260690646
C52	-0.8082416476	8.9999876220	12.8922911887
H53	-0.2416248366	8.2132528176	13.3925741721
H54	-1.8762445184	8.7566030771	12.9572032177
H55	-0.5447681920	9.0148681787	11.8301383924
C56	-1.2848650281	11.5392299893	12.8814392217
H57	-1.0435374360	11.6043039426	11.8158446426
H58	-2.3687113830	11.3855386959	12.9573324768
H59	-1.0346537656	12.4830000615	13.3686580106
Xpi	0.8980872288#	11.0664914856#	14.4057447337#

1 trans

C1	6.0597664592	7.9406349686	11.9964517522
H2	6.5863659123	7.1734354720	11.4200510213
C3	3.9404540378	7.2950738379	10.9068196859
H4	3.0900229811	7.6797402545	10.3385562363

N5	4.8903350062	8.3766609871	11.2152323043
O6	5.6051157091	10.7645241973	11.5355007646
O7	3.5905608448	10.2568828934	9.9220582603
P8	4.2535718818	9.9085607022	11.3461697575
Au9	2.5754487433	10.3859947730	12.9209924814
H10	4.4484161896	6.5463281516	10.2902152140
H11	3.5740562912	6.8073150237	11.8190551228
H12	5.7663828216	7.5083744249	12.9614277749
H13	6.7392741007	8.7760436564	12.1561361684
C14	5.5772747111	12.1689871607	11.8811632267
H15	5.1337416336	12.7542110711	11.0715803973
H16	6.6174907190	12.4609138694	12.0223361524
H17	5.0193259129	12.3266032641	12.8090901852
C18	4.3304890255	10.0964846135	8.6750040643
H19	4.3845147770	9.0401797404	8.4066696287
H20	5.3359846493	10.5116084586	8.7688656945
H21	3.7634303812	10.6481331879	7.9262846183
C22	1.4489744431	10.8545621990	14.8780790512
C23	0.4308252209	10.8845385485	13.9820642845
C24	2.1922665285	10.9218311584	15.9637029337
H25	3.2647174356	10.7495865112	15.8847983270
C26	1.6874256546	11.2660874841	17.3518281407
H27	1.8636513878	12.3412760248	17.4957552879
H28	0.6033765055	11.1177667169	17.4112027226
C29	2.4172589831	10.5097253174	18.4787877074
H30	3.5006445346	10.6095912620	18.3296197671
H31	2.1894184912	11.0175848754	19.4230221683
C32	2.0654190276	9.0128116412	18.6433624501
H33	0.9985904699	8.9306304137	18.8937468010
H34	2.6164058666	8.6370512891	19.5132887484
C35	2.3636058023	8.1412883133	17.4505179700
H36	1.6546762717	8.1875693966	16.6250459242
C37	3.4301672314	7.3321917545	17.3506911875
H38	4.1449742969	7.3195225982	18.1748187737
C39	3.7631041307	6.4373470554	16.2288216105
C40	4.4847096401	4.6844862439	14.1345334946
C41	5.0752080192	5.9437513593	16.1125645634
C42	2.8165913977	6.0213894141	15.2739507224
C43	3.1728447467	5.1567292213	14.2411769602
C44	5.4349548604	5.0824221957	15.0765393244
H45	5.8185608056	6.2360317340	16.8505442626
H46	1.7826541913	6.3402147333	15.3685684186
H47	2.4167355984	4.8221975682	13.5353849789
H48	6.4531716371	4.7078715098	15.0159602922
H49	4.7555565383	3.9932765161	13.3413185244
X50	1.1525509211#	9.8363232163#	13.8946323798#
C51	-0.4396008290	9.6683719602	13.7234735247
H52	-0.0102682139	8.7589731117	14.1464573811
H53	-1.4191187401	9.8411640208	14.1869662675
H54	-0.6114935343	9.5227526878	12.6524636179
C55	-0.0262992660	12.1914463793	13.3582109245
H56	-0.1753253091	12.0878007299	12.2789288236
H57	-0.9961521063	12.4601360463	13.7949829088
H58	0.6771203970	13.0035659939	13.5484255560

TS1 trans

C1	4.8248668918	8.9384838048	11.5991712416
H2	5.8770480145	8.7522964500	11.8547479889
C3	5.3785078629	10.7122055518	9.9730342387
H4	5.1270564534	10.0419188734	9.1441745706
N5	4.6123690701	10.3181477907	11.1636470329
O6	5.3296788490	12.3766342715	12.5745519475
O7	3.2562380764	12.5562721973	11.2504502092
P8	4.0252178283	11.4766695294	12.2028497396
Au9	2.7566834348	10.6960343676	14.0733586701
H10	5.1216409551	11.7323329143	9.6843741068
H11	6.4584885729	10.6574231544	10.1570852720
H12	4.5386358720	8.2528358366	10.7936113493
H13	4.2079643710	8.7179645157	12.4744174901
C14	5.1766294973	13.6141765933	13.2959123104
H15	4.6841888263	14.3624403483	12.6699844857
H16	6.1827717839	13.9481856784	13.5525283179
H17	4.5972921308	13.4604964222	14.2145338677
C18	1.9375205077	12.2560041765	10.7561400340
H19	1.2505330649	12.0435173338	11.5826196358
H20	1.9655542946	11.4040102528	10.0696377098
H21	1.6003528164	13.1449260960	10.2224377796
C22	1.6616982362	10.1196280363	15.7508470894
C23	0.5490111795	9.3322975963	15.6605093907
C24	2.1716998480	10.7053422487	17.0372936135
H25	3.1126175415	11.2240683360	16.8364485072
C26	1.3070227627	11.7076354675	17.8420802113
H27	1.3031117312	12.6729652543	17.3258443764
H28	0.2702064210	11.3669701477	17.9071062385
C29	1.9539353319	11.7661021568	19.2268216760
H30	2.9003388559	12.3196366427	19.1762487272
H31	1.3305461484	12.2650028819	19.9742408370
C32	2.2149012411	10.2906891965	19.5761749583
H33	1.3076792324	9.8286662977	19.9792730072
H34	2.9940490839	10.1630956567	20.3343735821
C35	2.5694772639	9.5642990797	18.2463822900
C36	3.9627234752	9.3031644567	18.0241652336
H37	1.9501693002	8.6910761986	18.0640267907
C38	-0.2942079739	8.8346890033	16.8177301768
H39	-1.3560451925	9.0142125127	16.6089787184
H40	-0.0702436014	9.2914131230	17.7796400155
H41	-0.1969801021	7.7443767558	16.9274729475
C42	0.0145255115	8.8447773782	14.3341276738
H43	0.6441282014	9.1473913752	13.4949861197
H44	-0.9988306488	9.2319579569	14.1643440224
H45	-0.0713870945	7.7493272586	14.3260724014
C46	5.7644897200	6.3395236731	15.6349622451
C47	4.3668398271	6.3648408312	15.7443880817
C48	3.7490155105	7.3247059197	16.5285165937
C49	4.5342312660	8.2949475276	17.2151615644
C50	5.9515991879	8.2557584908	17.0781351888
C51	6.5573555301	7.2852462202	16.3004490943
H52	6.2403207354	5.5726425830	15.0300174981
H53	3.7712102677	5.6228442685	15.2225229478
H54	2.6697511524	7.3389743476	16.6171279829
H55	6.5534485959	8.9979788543	17.5955414719
H56	7.6378123011	7.2539944589	16.2053602699
H58	4.6666977448	10.0069910775	18.4726491062

2 trans

C1	4.6210516933	8.2752801386	12.2182237445
H2	5.5765693930	7.9083047794	12.6121810313
C3	5.6958071651	9.7971829933	10.5870802730
H4	5.4107698444	9.1288241670	9.7675510401

N5	4.7484396557	9.6379128825	11.6999585195
O6	5.4679769671	11.8306789046	12.9002419481
O7	3.5535827608	11.9627342183	11.3657169322
P8	4.1508547275	10.9557703158	12.5059759898
Au9	2.5707083869	10.5542866063	14.3880316626
H10	5.6774704606	10.8243193984	10.2200808694
H11	6.7168457810	9.5532454092	10.9033898225
H12	4.2935576353	7.6053078470	11.4155582141
H13	3.8785217903	8.2386071281	13.0191244159
C14	5.3487058734	13.2240877795	13.2616420666
H15	5.0349766409	13.8158504852	12.4000063060
H16	6.3392389560	13.5395488948	13.5910777104
H17	4.6307458309	13.3563225529	14.0801427745
C18	2.3205551905	11.6461178053	10.6934853096
H19	1.4868068854	11.6040614257	11.4031811099
H20	2.4012516905	10.6949904026	10.1583768598
H21	2.1438554834	12.4520805322	9.9808750230
C22	0.9936150599	10.5103646389	15.7685121185
C23	-0.2554476791	10.3861144461	15.2891173025
C24	1.5153838465	10.6970537507	17.1861164015
H25	1.8593173359	11.7414474200	17.2777371132
C26	0.7144820778	10.3534412504	18.4623269083
H27	-0.0115808191	11.1228700395	18.7340514757
H28	0.1653601354	9.4174958829	18.3142560869
C29	1.8006115421	10.1755191974	19.5666436879
H30	1.8403147503	11.0451249565	20.2283352440
H31	1.5764615829	9.3119559840	20.1988245189
C32	3.1649063285	9.9987250031	18.8297944184
H33	3.7551657747	9.1591604705	19.2062912771
H34	3.7810032110	10.8997196815	18.9312756616
C35	2.7505834280	9.8022335278	17.3474474563
C36	3.8199080321	10.1384905975	16.3550605937
H37	2.4219814618	8.7664292509	17.2081242955
C38	-1.5193041384	10.4531158372	16.1241504168
H39	-2.2078596048	11.1848769299	15.6839012439
H40	-1.3514040883	10.7343057495	17.1601318066
H41	-2.0386429931	9.4862825781	16.1086901418
C42	-0.5615271318	10.1672371589	13.8194218651
H43	0.3329896571	10.0874111742	13.1904371550
H44	-1.1801450507	10.9838105490	13.4267677105
H45	-1.1335639320	9.2406191406	13.6835578100
C46	7.0460852584	7.5100199426	15.4737191805
C47	5.8228937473	6.9765810406	15.9013417578
C48	4.7478197540	7.8161523395	16.1530525384
C49	4.8792330414	9.2176953385	15.9920939073
C50	6.1166193167	9.7349498014	15.5381689665
C51	7.1895056287	8.8891632683	15.2882265322
H52	7.8863904858	6.8482539115	15.2841993095
H53	5.7170892242	5.9049529895	16.0386009342
H54	3.8040613833	7.3931005580	16.4795979983
H55	6.2242495810	10.8051902973	15.3924656775
H56	8.1381176250	9.2988844229	14.9559479733
H58	4.1302184125	11.1857219423	16.3769795346

TS2 trans

C1	1.4425043875	10.0495915443	9.2815628297
H2	1.5575986671	9.4441645203	8.3731465793
C3	3.3923288453	11.4869925237	8.7869725187
H4	2.7204963012	12.3193181302	8.5532713877
N5	2.7259781212	10.5860945284	9.7408204506
O6	4.7979976941	9.0580841782	10.1141043634
O7	4.5034195797	10.9844004027	11.6280404452
P8	3.6129809839	9.8218630150	10.9144936369
Au9	2.4028581192	8.4740930753	12.4359617656
H10	4.3063525526	11.8888098730	9.2269169324
H11	3.6462153226	10.9650198455	7.8565036267
H12	0.7621942275	10.8794928675	9.0640288548
H13	0.9892293284	9.4314401814	10.0607121374
C14	5.8580862065	8.3880163725	10.8251169537
H15	6.5567716723	9.1206480327	11.2367801887
H16	6.3671492007	7.7575799952	10.0958136420
H17	5.4537306451	7.7631802695	11.6302455430
C18	3.8843690488	11.9166899767	12.5330828282
H19	3.3276253219	11.3902388150	13.3168592484
H20	3.2115628716	12.5903724562	11.9942452466
H21	4.6945630393	12.4898370305	12.9847277327
C22	1.3187874917	7.3870991262	13.9322031777
C23	0.3271272171	6.5307207393	13.5184996657
C24	1.4276549956	8.0365710799	15.3201967116
H25	2.2849909681	8.7235373621	15.2661119436
C26	0.2724552733	8.8768798623	15.9034406850
H27	0.1170570824	9.8010638089	15.3382922995
H28	-0.6750908655	8.3319861954	15.8849047126
C29	0.7205502069	9.1317130232	17.3574400633
H30	1.3420824797	10.0322581055	17.4045616324
H31	-0.1242968248	9.2971436842	18.0319251740
C32	1.5627116119	7.8896697481	17.7755240715
H33	1.0634762266	7.2795385380	18.5329801311
H34	2.5190456810	8.1968121321	18.2120948995
C35	1.7828920491	7.0482392445	16.4671572282
C36	3.1971716472	6.5417233203	16.4339197144
H37	1.0804674261	6.2093434489	16.4475518301
C38	-0.8778053484	6.1061449948	14.3242879456
H39	-0.9751615381	5.0139152510	14.3086160600
H40	-1.7917544682	6.4999218194	13.8591915128
H41	-0.8626586601	6.4349395312	15.3607471553
C42	0.3615179067	5.8930913333	12.1502600063
H43	1.2982855026	6.0890536263	11.6231635495
H44	-0.4592179190	6.2838163580	11.5346829187
H45	0.2066828776	4.8096386236	12.2179543634
C46	4.6105439513	3.3804213088	18.9307138924
C47	3.2399176526	3.4945697205	18.6850394448
C48	2.7589612986	4.5145650087	17.8690780858
C49	3.6473583013	5.4408668856	17.2920300683
C50	5.0263007477	5.3149063703	17.5518061952
C51	5.5049015929	4.2914906494	18.3618866669
H52	4.9818183280	2.5823229709	19.5668576759
H53	2.5471211899	2.7878695394	19.1312416187
H54	1.6913646663	4.5916329213	17.6890814018
H55	5.7178538614	6.0277492163	17.1102820989
H56	6.5696684533	4.2041495257	18.5552989195
O57	3.5213815548	5.9782284626	14.6555086077
H58	3.9307759609	7.3402396739	16.3377022099
C59	3.3909171505	4.5750695687	14.4314925011
H60	3.6983520957	4.3780512365	13.3990137306
H61	4.0529385035	4.0251867519	15.1049090500
H62	2.3608172968	4.2228384100	14.5745375456
H63	2.5410012961	6.5938894390	13.9873103347

3 trans

H1	1.8429595072	10.6304293002	15.3903789875
C2	1.1469044935	10.4592528061	16.2135627731
C3	-0.1721865866	10.3384389479	15.7925498995
C4	1.7563672664	10.7779710914	17.5647442754
H5	1.8545173385	11.8764081550	17.5640112006
C6	1.0255628520	10.3432293158	18.8564110201
H7	0.1964164263	11.0089640481	19.1094087354
H8	0.6084056167	9.3363485665	18.7243795189
C9	2.1141541549	10.3211242821	19.9667921963
H10	1.9178067011	11.0661016425	20.7424549143
H11	2.1276106304	9.3466472732	20.4644439959
C12	3.4543367800	10.5956537772	19.2476781447
H13	4.2884056211	10.0549867795	19.7018573478
H14	3.6948931465	11.6618680205	19.2938771950
C15	3.2046238078	10.2265990670	17.7717588788
C16	4.2413631471	10.7338122281	16.7423898612
H17	3.1494339816	9.1304750875	17.6750238486
C18	-1.3923879613	10.3584894959	16.6804712107
H19	-1.8179271657	11.3708394159	16.6559305130
H20	-1.1908015803	10.1024960967	17.7166914552
H21	-2.1630548587	9.6858097116	16.2914604404
C22	-0.4867899317	10.4501269889	14.3131101626
H23	0.4053759742	10.3860200134	13.6856625526
H24	-0.9605069650	11.4237748884	14.1309568385
H25	-1.2035882004	9.6878526224	13.9919758116
C26	7.7677174002	8.2902146543	16.0581550994
C27	7.0576586242	8.1377613170	17.2485841236
C28	5.9214590100	8.9132372331	17.4963261603
C29	5.4745095383	9.8514241796	16.5565862696
C30	6.1988101943	9.9901834714	15.3613043307
C31	7.3346063909	9.2222627540	15.1124631956
H32	8.6535979985	7.6907865668	15.8688963216
H33	7.3920951496	7.4209086790	17.9935639896
H34	5.3911190608	8.7799573927	18.4331005010
H35	5.8676636891	10.7169751204	14.6227249530
H36	7.8807424882	9.3492827402	14.1820227587
H37	3.7499635599	10.7257386153	15.7603138484
Au38	0.9159509485	8.1432765119	15.9393488559
P39	1.2990897766	5.8349346753	15.7643931880
O40	1.0961654193	5.2444211209	17.2464440042
N41	0.3465228141	4.9051493229	14.7528067973
O42	2.7614939684	5.4417084033	15.2196078943
O43	4.5248706478	12.1253252526	16.9463990692
C44	5.7374565191	12.4798250968	17.6064094060
H45	5.6950729313	13.5635828083	17.7371478522
H46	5.8415371515	12.0083736998	18.5914631133
H47	6.6197825079	12.2285714061	17.0068804438
X48	0.4667851366#	10.2831833056#	15.7603141115#
C49	3.9498243588	6.1759581573	15.6091101082
C50	-1.0990149830	4.9245393812	15.0239144450
C51	0.6830329984	4.7332730823	13.3310550430
C52	1.2763534489	3.8282374050	17.5426153485
H53	0.2214611778	3.8050905953	12.9808590458
H54	0.3042151661	5.5612035163	12.7152941697
H55	1.7612805037	4.6508951591	13.2053863445
H56	-1.5315402329	3.9740555553	14.6974015404
H57	-1.2890369653	5.0332729945	16.0941750802
H58	-1.6077305183	5.7390429026	14.4889277580
H59	1.2335927234	3.7500122398	18.6280847420
H60	0.4754466735	3.2433806823	17.0874230728
H61	2.2457669984	3.4842318120	17.1764539192
H62	4.7646170135	5.7549419844	15.0213579110
H63	3.8425285369	7.2396014438	15.3805005785
H64	4.1523715588	6.0403374365	16.6738583554

1 cis

C1	0.2426125918	10.4397641997	15.1050767038
C2	-0.2704827778	9.2513935420	14.6835657999
C3	1.1154078143	11.4033226493	15.3228910788
H4	2.0932474642	11.2576516594	14.8583952581
C5	0.9165658957	12.7026879374	16.0683883425
H6	0.6762288374	13.4744145611	15.3231618773
H7	0.0421958881	12.6251544707	16.7273096252
C8	2.1405040433	13.1877050171	16.8709878377
H9	3.0042610720	13.2663370687	16.1966423623
H10	1.9287347083	14.2083842571	17.2090268959
C11	2.5220387582	12.3306009142	18.0970124220
H12	1.6505733617	12.2084624461	18.7538151979
H13	3.2643613967	12.9011403912	18.6739424372
C14	3.0998106964	10.9871364616	17.7496927323
H15	3.9613213855	11.0098553561	17.0815202169
C16	2.6506219308	9.8103191411	18.2127088605
H17	1.8048833876	9.8259299247	18.9027360528
C18	3.1617623571	8.4659545485	17.8995247151
C19	4.0399147777	5.8369199477	17.3568429681
C20	2.5906430654	7.3574314661	18.5508525408
C21	4.1871097549	8.2238623811	16.9647112738
C22	4.6191467347	6.9275923367	16.7002699195
C23	3.0230003409	6.0584481947	18.2852751243
H24	1.8062644975	7.5227519436	19.2867336233
H25	4.6543867456	9.0530737770	16.4416251097
H26	5.4149735205	6.7641442684	15.9788633867
H27	2.5695029413	5.2210872476	18.8084291019
H28	4.3826895638	4.8277366936	17.1485972773
C29	-0.0390496271	7.9749213007	15.4664414359
H30	0.3985681422	8.1634806840	16.4468633262
H31	-0.9636200513	7.3984856819	15.5747060943
H32	0.6620596418	7.3526336277	14.8950712011
C33	-0.9058799568	9.1032690362	13.3143744843
H34	-0.2145597693	8.5263620762	12.6862109297
H35	-1.8427180848	8.5394543170	13.3614171942
H36	-1.0850183305	10.0672034994	12.8358470539
X37	0.2868971780#	11.0253365713#	14.9519365043#
Au38	-1.8767909367	10.6120628786	15.9210052533
P39	-3.8721029352	11.3273363399	16.9361466767
O40	-4.0521083767	11.0113540170	18.5122750695
N41	-4.0999039026	12.9654907114	16.9334697601
O42	-5.0475130538	10.4989419750	16.1819723097
C43	-4.9429139322	13.6872792784	17.9004267560
C44	-3.6692044550	13.7670213765	15.7821335555
C45	-3.8898534860	9.6631014023	19.0086156465
C46	-6.4530487953	10.7407130094	16.4523607336
H47	-7.0036446354	10.0005701156	15.8730170423
H48	-6.6711975981	10.6178176582	17.5164156020
H49	-6.7318397622	11.7458239826	16.1251348865
H50	-4.0747705320	9.7143484377	20.0811841697
H51	-4.6060313015	8.9845284143	18.5377971120

H52	-2.8681617649	9.3136359402	18.8278908374
H53	-4.5225369066	14.0716291474	15.1640420265
H54	-3.1567375674	14.6668366025	16.1383942750
H55	-2.9735528044	13.2025144998	15.1552150438
H56	-5.8688266350	14.0365795187	17.4273136623
H57	-5.1866214874	13.0467198844	18.7462621514
H58	-4.3924344839	14.5573736965	18.2730590489
Xpi	-2.8817359941#	11.781292764 3#	17.4841640172#

TS1 cis

C1	0.2332242642	8.8626813632	15.9763884106
C2	1.3436148237	8.4117020949	16.6548096159
C3	0.0891951274	8.5593253627	14.5643188420
H4	0.8201368595	7.8481882331	14.1736289552
C5	-1.2600370315	8.3196659355	13.9174822490
H6	-1.6132269734	7.3286459671	14.2330639938
H7	-1.9949527648	9.0503845459	14.2756854735
C8	-1.0658340439	8.4053654408	12.4025890337
H9	-0.4599178500	7.5588700775	12.0574402078
H10	-2.0110206368	8.3667960568	11.8541580257
C11	-0.3212917798	9.7340698131	12.1621004086
H12	-1.0459571220	10.5556993702	12.1270895665
H13	0.2082136331	9.7376456005	11.2038088648
C14	0.6586311299	9.9876516012	13.3094672635
H15	1.6649185872	9.5943609217	13.1766781524
C16	0.5581320426	11.1865071072	14.0220364512
H17	-0.3745734632	11.7402544732	13.9111135073
C18	1.4757413422	11.7343901200	14.9670352742
C19	3.1719442660	12.8624900890	16.8952149926
C20	1.0982703661	12.9070462052	15.6704128894
C21	2.7292525275	11.1407641156	15.2597951831
C22	3.5657584322	11.7055901352	16.2126108481
C23	1.9366623420	13.4637082013	16.6230107638
H24	0.1388299788	13.3679471588	15.4520593341
H25	3.0548456088	10.2615221512	14.7159748722
H26	4.5320641793	11.2571834091	16.4216318757
H27	1.6405033004	14.3637778166	17.1523212013
H28	3.8340858969	13.3029722675	17.6350678041
C29	2.5183512112	7.6750739456	16.0467161003
H30	3.4579995819	8.0654267606	16.4540233758
H31	2.4805254264	6.6159060960	16.3339490573
H32	2.5803134582	7.7187888267	14.9583961662
C33	1.4872515770	8.5689138540	18.1460284537
H34	1.7883507962	7.6216995107	18.6105419256
H35	2.2835425998	9.2922366414	18.3719496336
H36	0.5664233899	8.9166511194	18.6183465868
Au38	-1.2844144494	9.9375539008	16.9357471165
P39	-2.9962478880	11.1132312407	18.1243258769
O40	-2.4732214279	12.0950819982	19.3101108501
N41	-4.0172423433	12.0723429230	17.2266962575
O42	-3.9732705367	10.1587923564	19.0154747834
C43	-5.1099415412	12.8036656972	17.8853260663
C44	-3.6044466639	12.6241008348	15.9378292948
C45	-1.7133766303	11.5731923206	20.4176295241
C46	-4.6288315449	9.0307466334	18.4057101446
H47	-5.1390684196	8.5016376666	19.2107858082
H48	-5.3603127439	9.3640488522	17.6634436352
H49	-3.8997345000	8.3632748428	17.9334152258
H50	-1.3818661565	12.4358087905	20.9964905352
H51	-2.3385639152	10.9268711040	21.0382393276
H52	-0.8388491767	11.0165099899	20.0609451654
H53	-4.4584595516	12.6294981336	15.2516119633
H54	-3.2332876179	13.6539173682	16.0345036002
H55	-2.8168240961	12.0045615155	15.4998767401
H56	-5.9803276005	12.8243619707	17.2211949431
H57	-5.3909910390	12.2993803795	18.8108172153
H58	-4.8171428342	13.8346113261	18.1187227453
X59	-3.3240646143#	11.2890304675#	17.5005243447#

2 cis

C1	0.7041139861	11.3742452389	14.8922402394
C2	0.5250646119	11.7410782173	13.6110215515
C3	2.0066426674	11.2573587353	15.6464810898
H4	2.8556294428	11.2362782915	14.9519044428
C5	2.2977036633	12.3433697606	16.7084646720
H6	2.6121460963	13.2875014877	16.2548483623
H7	1.3863857910	12.5575819480	17.2825779183
C8	3.3849485913	11.7076683318	17.6022406213
H9	4.3795716527	11.9524716444	17.2160472313
H10	3.3468477381	12.0813024939	18.6291453658
C11	3.1636274282	10.1661181814	17.5254260196
H12	2.9052256185	9.7310336004	18.4964058097
H13	4.0647519141	9.6455969059	17.1888911251
C14	2.0285093254	9.9513480526	16.4633280218
H15	2.2380896666	9.0964614602	15.8182874680
C16	0.7246101349	9.7279584041	17.1990980691
H17	0.5740315262	10.3904043807	18.0528118365
C18	0.1577793226	8.4036903023	17.3933368635
C19	-0.8740053244	5.8434727986	17.9007734055
C20	-0.5833148633	8.1426644690	18.5703763771
C21	0.3495310346	7.3526755517	16.4640790385
C22	-0.1638322060	6.0894070360	16.7180331142
C23	-1.0831081240	6.8712804594	18.8248543848
H24	-0.7550089248	8.9488848250	19.2766662668
H25	0.8895388696	7.5354873886	15.5412413863
H26	-0.0112254442	5.2888312396	16.0010145555
H27	-1.6312051731	6.6760876120	19.7414253419
H28	-1.2644949508	4.8493683342	18.0988463392
C29	1.6634581451	12.0993632909	12.6763435615
H30	2.6520570283	12.0144141890	13.1285308596
H31	1.6391128967	11.4548822733	11.7885528511
H32	1.5459716982	13.1301926564	12.3196764721
C33	-0.8323720189	11.8429985802	12.9472549492
H34	-0.9869599546	12.8495843985	12.5392989921
H35	-0.9031240083	11.1440275985	12.1043700509
H36	-1.6665068458	11.6258268632	13.6244944536
X37	0.6139120437#	11.0920537236#	14.4365412172#
Au38	-0.9505228847	10.9074832325	16.0560759942
P39	-3.1149234003	10.8186199107	17.2656206456
O40	-3.9698858665	12.2053752106	17.1811567179
N41	-4.2714174961	9.7535132493	16.7316706426
O42	-2.7965684622	10.6572143747	18.8671281707
C43	-5.7121648891	9.8898930641	16.9831076811
C44	-3.8782995509	8.4940530477	16.0953455588
C45	-3.3527873799	13.4529348959	17.5605784295
C46	-3.8475225785	10.6320292328	19.8611396215
H47	-3.3551139687	10.6624329355	20.8337316026

H48	-4.5072375959	11.4978000308	19.7577632340
H49	-4.4305392615	9.7106714072	19.7739114539
H50	-4.0938229912	14.2286805911	17.3675215653
H51	-3.0836534237	13.4528828776	18.6208497214
H52	-2.4602344757	13.6433769966	16.9546565980
H53	-4.0893448513	7.6352523924	16.7449610731
H54	-4.4326874385	8.3655656372	15.1584568682
H55	-2.8101288837	8.4953992890	15.8630412728
H56	-6.0651279621	9.1169845893	17.6776377701
H57	-5.9357222814	10.8745899393	17.3914016809
H58	-6.2569387272	9.7809397644	16.0386635951
X59	-2.96756869977#	11.2107969268#	17.3003097727#

TS2 cis

C1	0.3401565350	10.1729211248	15.3016174797
C2	-0.4129115098	9.4577730699	14.3904605737
C3	1.4364595344	11.2057305001	15.0480542842
H4	1.6857258486	11.3313364227	13.9878503077
C5	1.3555206158	12.5886327878	15.7337008391
H6	0.9405602360	13.3611602940	15.0791684874
H7	0.7118087434	12.5371581748	16.6233283234
C8	2.8086719012	12.8527427901	16.1681030976
H9	3.4105985106	13.1356015023	15.2958245305
H10	2.8960398073	13.6631582310	16.8978836807
C11	3.2845842264	11.4895704086	16.7198130475
H12	3.0120676595	11.3927723811	17.7781142651
H13	4.3695725033	11.3668957827	16.6598932515
C14	2.5245484176	10.4352098625	15.8685415579
H15	3.1991347420	9.8753111853	15.2168938283
C16	1.5938147031	9.4661185979	16.6384898420
H17	1.2531593794	9.8757743789	17.5888288397
C18	1.7897195893	8.0035814380	16.6968710762
C19	2.1110197814	5.2145654266	16.8947789919
C20	1.3263137606	7.3003363503	17.8239014434
C21	2.4204717810	7.2782501415	15.6702556754
C22	2.5809605166	5.8987556582	15.7711055186
C23	1.4830270678	5.9201074023	17.9231502119
H24	0.8446717257	7.8472267713	18.6315943835
H25	2.7880522438	7.7913827201	14.7866673190
H26	3.0751160773	5.3534631544	14.9724812367
H27	1.1227950313	5.3958405272	18.8035231839
H28	2.2373437412	4.1384393416	16.9699439670
C29	-0.6013864711	9.9425192682	12.9738039076
H30	-0.3022366873	10.9827680068	12.8382121691
H31	0.0025782050	9.3180001195	12.3011847745
H32	-1.6428384368	9.8264974953	12.6579905068
C33	-0.9722325380	8.0908669272	14.6956604120
H34	-2.0179328686	8.0066365907	14.3825499391
H35	-0.4067297207	7.3500729548	14.1134720439
H36	-0.8832012437	7.8263609859	15.7492396873
Au37	-1.4886662692	10.7907859928	16.2803180745
P38	-3.2847818435	11.5990259943	17.5676883482
O39	-2.8921231690	12.3845578739	18.9325159974
N40	-4.2542705279	12.7345387519	16.8498091369
O41	-4.0987368910	10.2776496023	18.0582092588
C42	-5.0730164574	13.7103495812	17.5853545451
C43	-4.5466802551	12.6543567361	15.4151390197
C44	-2.0423410173	11.7498346349	19.9111500921
C45	-5.3329968695	10.3722316381	18.8117805672
H46	-5.6035675828	9.3516286244	19.0807487283
H47	-5.1937944954	10.9696116532	19.7170481678
H48	-6.1211775195	10.8097250658	18.1931849196
H49	-1.9097184531	12.4760100977	20.7129620734
H50	-2.5070521131	10.8412279850	20.3040549163
H51	-1.0683130093	11.5075965649	19.4722306580
H52	-5.5661200670	12.2916905828	15.2334896749
H53	-4.4444257107	13.6480627209	14.9662668255
H54	-3.8451064806	11.9804235206	14.9164039327
H55	-6.1386115690	13.4571165325	17.5195283192
H56	-4.7731273053	13.7482368118	18.6312722142
H57	-4.9242843905	14.7033256177	17.1479107044
X58	0.0038336887#	9.7808565887#	14.9204134360#

3 cis

C1	0.8421140115	10.1340284918	15.9461875734
C2	0.3554581721	10.5421032629	14.7110209311
C3	1.9486795034	10.7438871320	16.8078132546
H4	2.7119719868	11.2743557925	16.2300193027
C5	1.6177056082	11.5039687636	18.1171231302
H6	1.7889078777	12.5811793106	18.0316443853
H7	0.5622963049	11.3662912183	18.3890402035
C8	2.5133476500	10.8138417338	19.1647817172
H9	3.5473969385	11.1616893615	19.0515939352
H10	2.2097080225	11.0326830179	20.1931547381
C11	2.4202027174	9.3128655683	18.8105732270
H12	1.5247361713	8.8699482640	19.2646038267
H13	3.2775613575	8.7414921038	19.1767917764
C14	2.3121364271	9.2924313724	17.2685906643
H15	3.2027821739	8.8889638826	16.7832587043
C16	1.0008281198	8.7356876853	16.6000717525
H17	0.2409403835	8.5773681113	17.3737899998
C18	1.0796948721	7.5008318757	15.7350688429
C19	1.2195351530	5.1769025415	14.1568646154
C20	0.1898733218	6.4390768899	15.9423091903
C21	2.0460337252	7.3777259586	14.7251071223
C22	2.1155162137	6.2265687228	13.9428064017
C23	0.2571543738	5.2850726565	15.1600329932
H24	-0.5586410194	6.5120241645	16.7284363472
H25	2.7532225923	8.1843975786	14.5464127967
H26	2.8713528537	6.1466525996	13.1667104638
H27	-0.4385078036	4.4702515393	15.3384981166
H28	1.2758047790	4.2796281462	13.5477530753
C29	0.7907538982	11.8676371373	14.1189078854
H30	1.1852041117	12.5573529642	14.8671570405
H31	1.5775719608	11.6813363940	13.3753603892
H32	-0.0328619716	12.3572882269	13.5907124421
C33	-0.3561803913	9.6100950652	13.7509367794
H34	-1.1646763737	10.1316544845	13.2290513977
H35	0.3575025633	9.2762548970	12.9863926691
H36	-0.7587408711	8.7214237288	14.2360771342
X37	0.7041139861#	11.3742452389#	14.8922402394#
Au38	-1.3072377946	11.0364430314	16.3421917019
P39	-3.2936283596	11.8123583410	17.3147789347
O40	-4.5140762602	12.1471720795	16.3055410206
N41	-4.0458605045	10.7707991200	18.3572263216
O42	-2.8932837141	13.2314225979	17.9959055836
C43	-5.4776495199	10.8284418161	18.6928451899
C44	-3.2596949929	9.8657737570	19.2012712937
C45	-4.3209781405	13.0481207286	15.1925934687

C46	-3.8358303971	14.0015507695	18.7846776014
H47	-3.3315873943	14.9352433389	19.0309713410
H48	-4.7443342319	14.2093631114	18.2132573730
H49	-4.0849514107	13.4642103004	19.7035019203
H50	-5.2809702991	13.1009080370	14.6798722782
H51	-4.0271476990	14.0420371892	15.5403193422
H52	-3.5623032483	12.6516422959	14.5100288146
H53	-3.2393030360	10.2059443466	20.2440723583
H54	-3.7002983640	8.8637237220	19.1686215321
H55	-2.2298868691	9.7982399786	18.8401633606
H56	-5.6240931557	11.1876259276	19.7188406532
H57	-6.0056595769	11.4818530843	18.0003478670
H58	-5.9043398091	9.8233197842	18.6108402862
X59	-3.1149234003#	10.8186199107#	17.2656206456#

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Au	-1.414892	-1.071412	-0.797133
C	-2.866739	-0.924932	-2.323963
C	-4.144126	-1.383767	-2.112868
C	-2.612570	-0.092395	-3.463708
H	-3.448652	0.113433	-4.133056
C	-1.328950	-0.139556	-4.246943
H	-1.359182	-0.966680	-4.969344
H	-0.470715	-0.292220	-3.580639
N	-1.138794	1.131150	-4.955192
C	-1.256339	2.192686	-3.938588
H	-0.255340	2.379832	-3.537089
H	-1.611863	3.113031	-4.407647
C	-2.158918	1.734649	-2.806439
C	-3.448086	2.224298	-2.651008
H	-3.898764	2.720137	-3.515931
C	-4.298720	1.915102	-1.553003
C	-6.056197	1.012790	0.421128
C	-5.689814	2.087112	-1.696295
C	-3.814734	1.328104	-0.368509
C	-4.690365	0.859834	0.596070
C	-6.558703	1.645928	-0.718606
H	-6.067329	2.549363	-2.605291
H	-2.746733	1.269368	-0.178594
H	-4.292150	0.368206	1.483369
H	-7.631070	1.775843	-0.837386
H	-6.745953	0.658342	1.187268
C	-5.294489	-1.237470	-3.057851
H	-5.482128	-2.184954	-3.562155
H	-6.203624	-1.008233	-2.506346
H	-5.171412	-0.493960	-3.835911
C	-4.520963	-2.186999	-0.906694
H	-3.724534	-2.227825	-0.156858
H	-5.419273	-1.758854	-0.422582
H	-4.799701	-3.219093	-1.193371
H	-1.631383	1.392519	-1.910869
C	-1.534897	-2.361589	2.679174
C	-2.427241	-1.629654	3.459987
C	-3.781864	-2.023728	3.524529
C	-4.830025	-1.109187	4.125391
H	-4.864830	-1.215576	5.220269
H	-4.548150	-0.062579	3.951690
C	-6.218434	-1.396543	3.574628
H	-6.963981	-0.764776	4.080846
H	-6.250078	-1.141321	2.501586
C	-6.536165	-2.871410	3.740680
H	-7.577356	-3.088284	3.474860
H	-6.422444	-3.141190	4.801154
C	-5.591760	-3.704112	2.881526
H	-5.628703	-4.764780	3.167902
H	-5.933237	-3.674759	1.832220
C	-4.159616	-3.227718	2.914255
C	-3.204692	-3.982387	2.231950
H	-3.514719	-4.911630	1.751695
C	-1.891301	-3.559614	2.050798
C	-1.615359	0.727510	3.284585
C	-1.971890	-0.357780	4.089595
C	-2.018912	-0.197193	5.488932
C	-2.244794	-1.405064	6.372625
H	-3.307725	-1.701124	6.331499
H	-1.686832	-2.261408	5.967264
C	-1.868850	-1.157992	7.829056
H	-2.203229	-2.003184	8.446169
H	-0.771342	-1.108570	7.930917
C	-2.478464	0.151180	8.306371
H	-2.327566	0.290660	9.385422
H	-3.569950	0.130546	8.138033
C	-1.858911	1.307727	7.532086
H	-0.821539	1.458088	7.880859
H	-2.383366	2.251197	7.743042
C	-1.838644	1.075646	6.040097
C	-1.697051	2.168718	5.182117
H	-1.700104	3.175427	5.603016
C	-1.598545	2.037077	3.800944
C	-1.021075	-4.235530	1.061841
C	-1.508650	-4.394862	-0.200413
H	-2.525283	-4.082383	-0.423834
C	-0.725672	-4.901768	-1.276793
C	-1.249391	-5.027036	-2.566135
H	-2.289227	-4.760519	-2.739767
C	-0.456682	-5.493729	-3.604178
H	-0.878472	-5.623950	-4.599161
C	0.878626	-5.791098	-3.388351
H	1.480920	-6.159810	-4.216715
C	1.454586	-5.636676	-2.118682
C	2.853292	-5.871022	-1.862468
C	3.307693	-5.854738	-0.578206
H	4.363392	-6.023409	-0.384848
C	2.469735	-5.531795	0.534959
C	2.949800	-5.521532	1.844957
H	3.974737	-5.827253	2.029616
C	2.130974	-5.128732	2.893612
H	2.511061	-5.140751	3.911559
C	0.835772	-4.699681	2.653350
H	0.209776	-4.372246	3.481109
C	0.314963	-4.683584	1.357635
C	1.129540	-5.149728	0.288694
C	0.626370	-5.231355	-1.034934
C	3.790428	-6.050341	-2.997463
C	4.766086	-7.046567	-2.973622
H	4.803745	-7.765906	-2.139383
C	5.686574	-7.148514	-4.022340
C	5.639415	-6.269383	-5.116021

H	6.349647	-6.358327	-5.938617
C	4.656534	-5.275784	-5.155761
C	3.755567	-5.156657	-4.107049
H	3.027740	-4.347902	-4.137051
C	6.698981	-8.257281	-3.952285
C	4.609900	-4.346590	-6.364620
C	-1.729390	3.220035	2.904296
C	-2.924020	3.368654	2.272096
H	-3.738450	2.687017	2.506265
C	-3.153326	4.357480	1.271399
C	-4.399946	4.538829	0.668738
H	-5.252155	3.964939	1.030708
C	-4.548116	5.435694	-0.377195
H	-5.529693	5.589052	-0.824179
C	-3.447451	6.126175	-0.875227
C	-2.182561	5.982343	-0.293001
C	-1.012506	6.685620	-0.773978
C	0.096401	6.742204	0.013247
H	0.985017	7.274290	-0.340543
C	0.200741	5.999521	1.234112
C	1.343034	6.044906	2.030470
H	2.145144	6.737059	1.768371
C	1.463812	5.203344	3.128433
H	2.355960	5.254464	3.746700
C	0.477294	4.268139	3.426721
H	0.602605	3.587055	4.268376
C	-0.686597	4.188315	2.661613
C	-0.846777	5.104423	1.583265
C	-2.052015	5.139214	0.841048
C	-0.997575	7.231004	-2.144689
C	-1.434641	6.436956	-3.206310
H	-1.831963	5.452320	-3.002124
C	-1.375629	6.889665	-4.513303
C	-0.874383	8.135252	-4.803900
H	-0.838160	8.487763	-5.829920
C	-0.437719	8.923026	-3.754869
C	-0.498930	8.477684	-2.438996
H	-0.179654	9.127147	-1.631722
C	-1.785285	5.991978	-5.631696
C	0.097543	10.300492	-3.990200
C	2.310903	-0.569732	0.685960
H	3.122473	0.156790	0.813052
C	2.698634	-1.837755	1.420543
H	2.892107	-1.621150	2.477127
H	3.599902	-2.275024	0.975951
H	1.912075	-2.598368	1.392172
C	2.172089	-0.763747	-0.812835
C	1.739815	-1.965075	-1.370675
H	1.446664	-2.793617	-0.729843
C	1.696366	-2.137370	-2.751875
H	1.328599	-3.077392	-3.156937
C	2.112664	-1.122166	-3.601604
H	2.102684	-1.268333	-4.683170
C	2.537978	0.082619	-3.057483
H	2.877625	0.885134	-3.709387
C	2.562600	0.257572	-1.678232
H	2.925707	1.195592	-1.264983
C	1.450044	1.363785	2.062259
H	0.491035	1.742644	2.436645
C	2.342991	1.133123	3.269049
H	1.849432	0.437763	3.962640
H	2.522225	2.079172	3.798587
H	3.319611	0.706470	3.002376
C	1.927346	2.382990	1.045148
C	1.011604	2.793166	0.069326
H	-0.006167	2.392717	0.097323
C	1.378092	3.691458	-0.926262
H	0.642492	4.015863	-1.666820
C	2.678184	4.196075	-0.965660
H	2.970983	4.904985	-1.743881
C	3.596230	3.798015	0.000873
H	4.612156	4.189071	-0.021183
C	3.220963	2.896831	1.004914
H	3.951626	2.596509	1.758733
N	1.146959	0.104286	1.341236
O	-0.294594	-1.772098	2.447123
O	-1.397676	0.522989	1.919754
F	7.636825	-8.148673	-4.911180
F	6.098132	-9.460224	-4.099594
F	7.304803	-8.247134	-2.750320
F	3.610023	-3.453435	-6.278154
F	5.755861	-3.642204	-6.499977
F	4.429999	-5.065953	-7.510373
F	-0.777597	5.226002	-6.034661
F	-2.221898	6.656271	-6.699788
F	-2.754806	5.162722	-5.252885
F	0.174558	10.584925	-5.294356
F	-0.684878	11.218115	-3.411484
F	1.336894	10.431887	-3.451031
P	-0.355011	-0.590391	1.281356
H	-3.575262	6.813022	-1.711810
S	-2.224012	1.354487	-6.267206
O	-2.251730	0.074080	-6.952200
O	-3.469093	1.943717	-5.795194
C	-1.433083	2.570623	-7.256835
C	-0.311837	4.348659	-9.049630
C	-2.202980	3.618391	-7.751075
C	-0.115997	2.389809	-7.647027
C	0.433100	3.283324	-8.535290
C	-1.636967	4.495537	-8.646701
H	-3.232870	3.736056	-7.436726
H	0.463279	1.552712	-7.263780
H	1.464347	3.151973	-8.846332
H	-2.232951	5.319369	-9.039257
C	0.298678	5.306477	-10.009865
H	1.098828	4.838583	-10.594427
H	0.741688	6.157469	-9.478536
H	-0.446317	5.703443	-10.705065

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Au	-1.023907	0.321829	0.562350
C	-2.432879	-0.496454	1.871416
C	-2.937361	-1.762378	1.626010
C	-3.022861	0.312766	2.889140
H	-3.836272	-0.122035	3.476136
C	-2.206020	1.285851	3.727016
H	-1.693508	0.735013	4.535442
H	-1.435644	1.790274	3.118718

C	-3.967922	2.822508	3.241555
H	-3.588155	3.811362	2.927575
H	-4.988367	2.977586	3.611950
C	-3.955057	1.868394	2.059492
C	-5.105759	1.244183	1.590064
H	-5.960962	1.186929	2.267448
C	-5.195751	0.510611	0.367321
C	-5.359936	-1.077018	-1.911064
C	-6.284958	-0.374838	0.164060
C	-4.200428	0.594626	-0.613003
C	-4.278562	-0.204942	-1.734644
C	-6.365671	-1.161085	-0.962873
H	-7.056915	-0.442448	0.921295
H	-3.381549	1.314556	-0.517431
H	-3.494309	-0.127795	-2.475637
H	-7.209424	-1.839981	-1.112376
H	-5.438087	-1.681417	-2.809920
C	-4.083090	-2.406460	2.351549
H	-3.695124	-3.111404	3.101481
H	-4.680578	-3.009619	1.653316
H	-4.755365	-1.716434	2.870660
C	-2.343429	-2.669057	0.593808
H	-1.319652	-2.385635	0.318348
H	-2.961178	-2.637266	-0.324462
H	-2.354135	-3.718119	0.924723
H	-3.155293	2.048202	1.335056
C	-1.153032	2.917257	-2.263760
C	-2.008631	2.462850	-3.265942
C	-3.362905	2.866556	-3.251995
C	-4.358114	2.266036	-4.217705
H	-4.271200	2.760042	-5.198773
H	-4.101707	1.210810	-4.403655
C	-5.800275	2.402256	-3.751074
H	-6.475429	2.070054	-4.548327
H	-5.980499	1.741984	-2.887061
C	-6.079850	3.844084	-3.354980
H	-7.141202	4.000021	-3.127398
H	-5.838591	4.507904	-4.199334
C	-5.229792	4.207417	-2.149829
H	-5.280331	5.285783	-1.941731
H	-5.648649	3.711346	-1.257194
C	-3.784515	3.784807	-2.278941
C	-2.864545	4.296209	-1.362793
H	-3.199722	5.045672	-0.643465
C	-1.536705	3.875574	-1.315417
C	-1.131487	0.194629	-3.833246
C	-1.519690	1.465575	-4.264369
C	-1.535068	1.732381	-5.651064
C	-1.699860	3.154062	-6.138398
H	-2.756065	3.460034	-6.069002
H	-1.153511	3.832992	-5.463571
C	-1.243732	3.337743	-7.581408
H	-1.511817	4.343205	-7.926911
H	-0.145997	3.265791	-7.641367
C	-1.869363	2.262537	-8.460800
H	-1.666392	2.443538	-9.525099
H	-2.965480	2.284624	-8.339738
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C	-1.338532	0.680574	-6.558976
C	-1.178361	-0.619022	-6.073839
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C	-0.955335	4.314904	1.040075
H	-1.929745	3.898347	1.308639
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H	-1.471065	4.323510	3.713223
C	0.441783	4.992867	4.446296
H	0.133677	4.957063	5.490724
C	1.746224	5.364395	4.129269
H	2.442613	5.615714	4.928651
C	2.175103	5.432429	2.796254
C	3.529662	5.786395	2.426333
C	3.823746	6.022012	1.114288
H	4.842393	6.299032	0.831199
C	2.867088	5.831188	0.070063
C	3.189964	6.074269	-1.269417
H	4.175889	6.473930	-1.515115
C	2.265642	5.811744	-2.271629
H	2.518163	6.024236	-3.309924
C	1.025686	5.262163	-1.963541
H	0.323031	5.044039	-2.766628
C	0.663713	4.980320	-0.638360
C	1.579704	5.319330	0.399181
C	1.230523	5.159205	1.766391
C	4.613258	5.831198	3.433587
C	5.500355	6.910149	3.501978
H	5.345371	7.779348	2.861525
C	6.578255	6.893397	4.385002
C	6.797712	5.799478	5.211040
H	7.643901	5.785398	5.895237
C	5.912289	4.725603	5.152824
C	4.829179	4.737542	4.278185
H	4.168370	3.867777	4.222548
C	7.479204	8.097790	4.424884
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C	-3.507022	-4.432516	-2.322039
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C	0.223322	-6.521531	-1.573423
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H	2.275732	-6.685184	-2.159359
C	1.247890	-5.180799	-3.351700
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H	3.207914	-3.540679	-5.592216
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H	1.243445	-2.011147	-5.628262
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C	0.101674	-7.662546	2.023703
C	0.938076	-8.782921	2.020869
H	1.124267	-9.335978	2.940766
C	1.530550	-9.173067	0.830314
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C	3.161387	2.142050	-1.075782
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H	2.361450	2.888703	-1.037693
C	2.258941	0.634101	0.766220
C	1.826338	1.733445	1.511244
H	1.746093	2.716961	1.047185
C	1.503320	1.601531	2.857556
H	1.175557	2.479998	3.419993
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H	1.375856	0.261462	4.538125
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H	2.163237	-1.710000	3.236507
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H	2.744221	-1.464245	0.859702
C	2.026610	-0.702012	-2.686214
H	1.127009	-0.928399	-3.260739
C	3.044964	-0.124125	-3.648021
H	2.631472	0.775113	-4.118377
H	3.280828	-0.851336	-4.437186
H	3.983900	0.151620	-3.162271
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C	1.425952	-2.648692	-1.263237
H	0.405240	-2.263279	-1.279846
C	1.716527	-3.771913	-0.516873
H	0.925767	-4.270277	0.043608
C	3.017084	-4.262830	-0.489318
H	3.250787	-5.149822	0.093872
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F	6.814503	9.174612	4.873027
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F	7.177365	3.615287	6.802336
F	5.037175	3.280355	6.770203
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F	0.414860	-6.800232	4.172826
F	-1.163685	-8.247477	3.912085
F	-1.379349	-6.217534	3.148712
F	2.724215	-10.858553	1.971448
F	1.925635	-11.343974	0.016530
F	3.611305	-10.008976	0.198009
P	0.064865	0.832858	-1.475963
H	-2.329426	-7.190852	-0.710515
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S	-3.963234	1.697980	5.669678
O	-2.973884	0.999215	6.501723
O	-5.157589	0.978993	5.187888
C	-4.479831	3.224676	6.425498
C	-5.289218	5.588776	7.696989
C	-5.835377	3.482938	6.635651
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H	-6.565307	2.757447	6.312313
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H	-3.187703	6.010917	7.795589
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